Nonparametric Methods for Density Estimation Nearest Neighbour Classification

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Probability Estimation

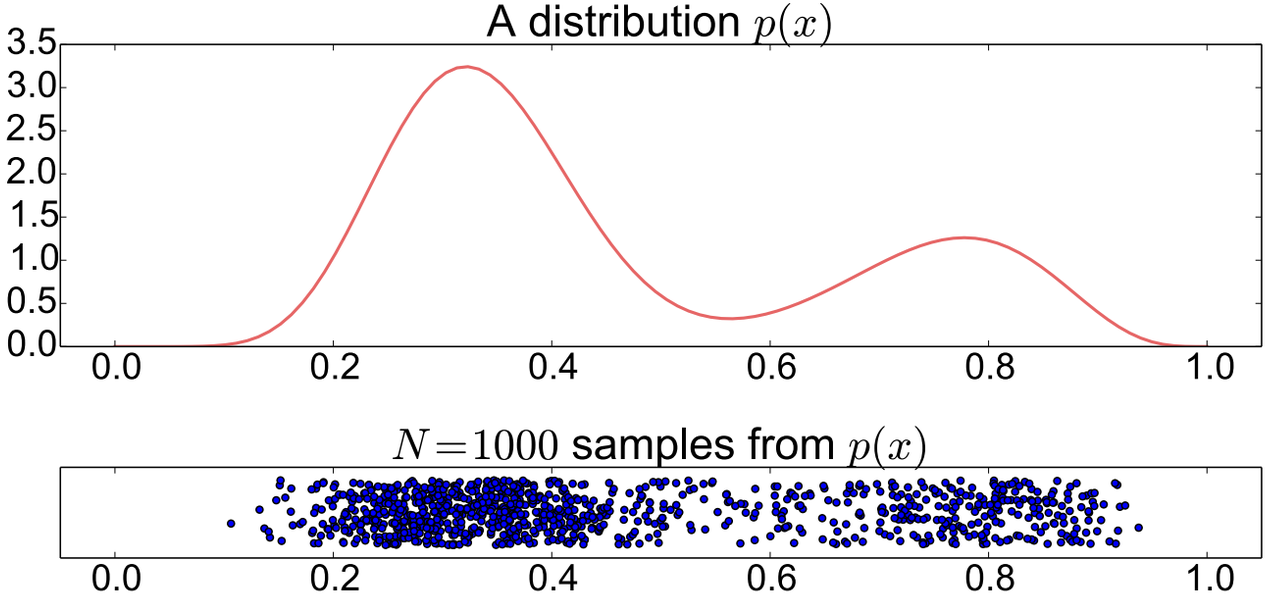
Recall that in the previous lecture, **parametric** methods for density estimation have been dealt with. The advantage of these methods is that there is a low number of parameters to estimate. The disadvantage is that the resulting estimated density can be arbitrarily wrong if the underlying distribution does not agree with the assumed parametric model.

Non-Parametric Density Estimation

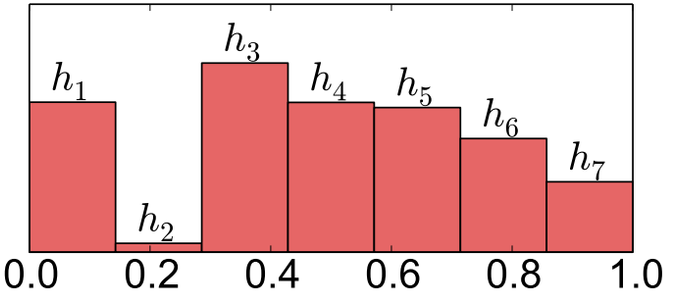
- histogram
- Parzen estimation
- Nearest Neighbor approach

Histogram (1)

Consider the following distribution on the interval $[0, 1]$, and i.i.d. sampling from it.
We will fit the distribution by a 'histogram' with B bins. More precisely, we will estimate a piecewise-constant function on the interval $[0, 1]$ with B segments of the same length. For a given B, the parameters of this piecewise-constant function are the heights $h_1, h_2, ..., h_B$ of the individual bins. This function is denoted $p(x|\{h_1, h_2, ..., h_B\})$.



$p(x|\{h_1, h_2, .., h_B\})$ to be estimated



For the given number of bins B, $h_1, h_2, ..., h_B$ must conform to the constraint that the area under the function must sum up to one,

$$\frac{1}{B}\sum_{i=1}^{B} h_i = 1\,, \qquad (h_i \geq 0.) \tag{1}$$

Histogram (2)

Let us estimate $\{h_i, i = 1, 2, ..., B\}$ by Maximum Likelihood (ML) approach. Let N_i denote the number of samples which belong the i-th bin (thus clearly, $\sum_{i=1}^{B} N_i = N$). The likelihood $p(\mathcal{T}|\boldsymbol{\theta})$ of observing the samples $\mathcal{T} = \{x_1, x_2, ..., x_N\}$ given the parameters $\boldsymbol{\theta} = \{h_1, h_2, ..., h_B\}$ is

$$p(\mathcal{T}|\boldsymbol{\theta}) = \prod_{j=1}^{B} h_j^{N_j} \,. \tag{2}$$

The maximization task is then

$$\sum_{j=1}^{B} N_j \log h_j \to \max \,, \qquad \text{subject to } \frac{1}{B}\sum_{j=1}^{B} h_j = 1 \,, \tag{3}$$

where maximization has been formulated using the log-likelihood. The Lagrangian of the optimization task and the conditions of optimality (using the derivative $\partial/\partial h_k$) are then:

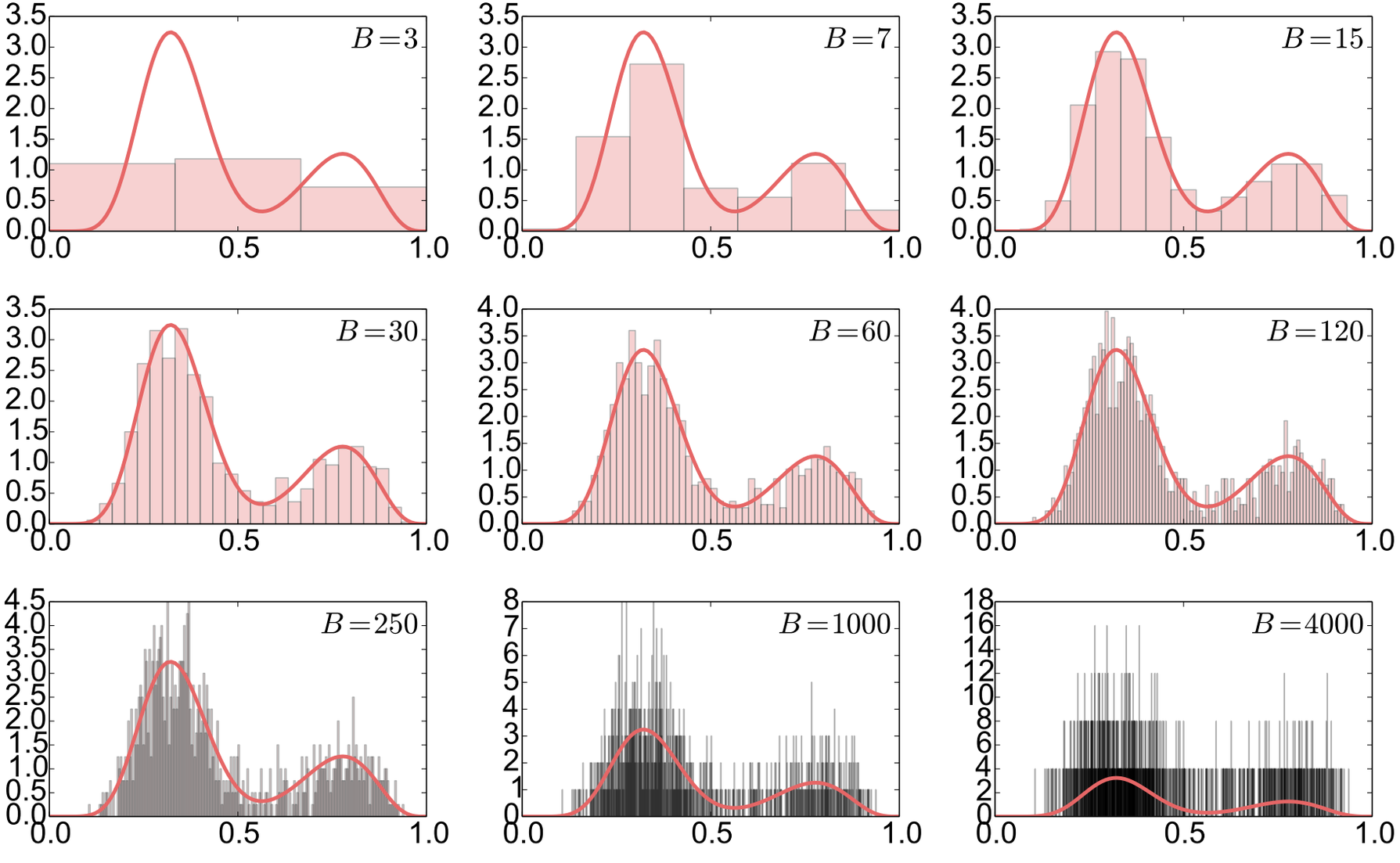
$$\text{Lagrangian: } \sum_{j=1}^{B} N_j \log h_j + \lambda \left(\frac{1}{B}\sum_{j=1}^{B} h_j - 1 \right) \tag{4}$$

$$\frac{N_k}{h_k} + \frac{\lambda}{B} = 0 \Rightarrow \frac{h_k}{N_k} = \text{const.} \Rightarrow \quad h_k = B\frac{N_k}{N} \quad . \tag{5}$$

Histogram (3)

$$h_k = B\frac{N_k}{N} \qquad (6)$$

This result is in line with the common use of histograms for approximating pdf's. Results for different B's:



Histogram: MAP and Bayes estimation

The ML estimation of h_i's suffers from similar problems as e.g. the Binomial Distribution estimation (recall estimating π, the fraction of red socks) in the last lecture.
MAP and Bayes estimation of h_i's need a suitable prior. The conjugate prior in this case is the Dirichlet Distribution, with the pdf $p(h_1, h_2, ..., h_B|\alpha_1, \alpha_2, ..., \alpha_B) \sim \prod h_i^{\alpha_i - 1}$.

MAP Estimation:

$$h_i = B\frac{N_i + \alpha_i - 1}{N + \sum_{i=1}^{B} \alpha_i - B} \tag{7}$$

Bayes Estimation:

$$h_i = B\frac{N_i + \alpha_i}{N + \sum_{i=1}^{B} \alpha_i} \tag{8}$$

Interpretation: The parameters α_i's again can be interpreted as 'virtual' observations, as if α_k points have already been assigned to the k-th bin.

Example: Take $\alpha_i = 2$ for all $i = 1, 2, ..., B$.

MAP:

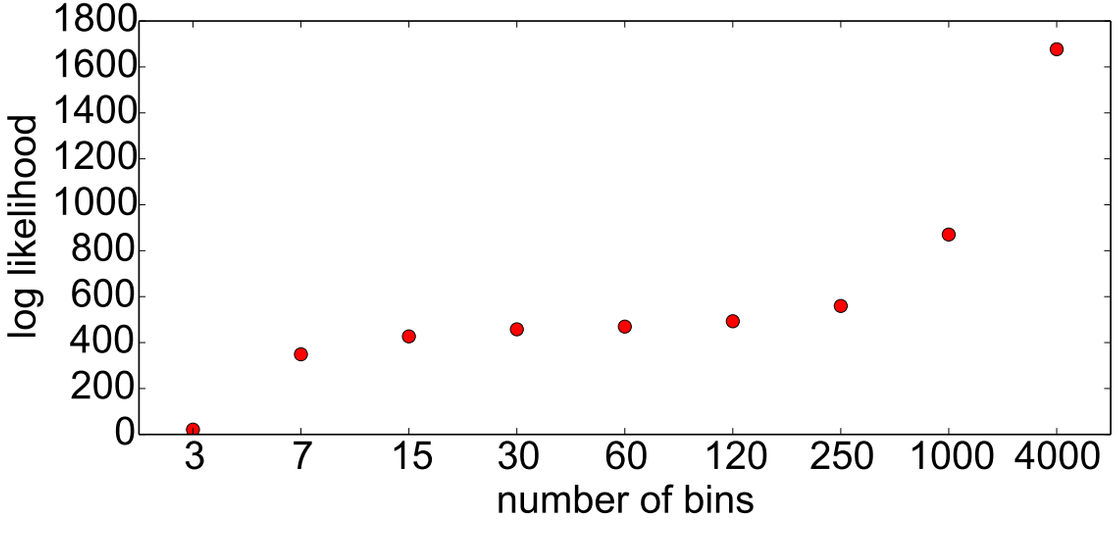
$$h_i = B\frac{N_i + 1}{N + B} \tag{9}$$

Bayes:

$$h_i = B\frac{N_i + 2}{N + 2B} \tag{10}$$

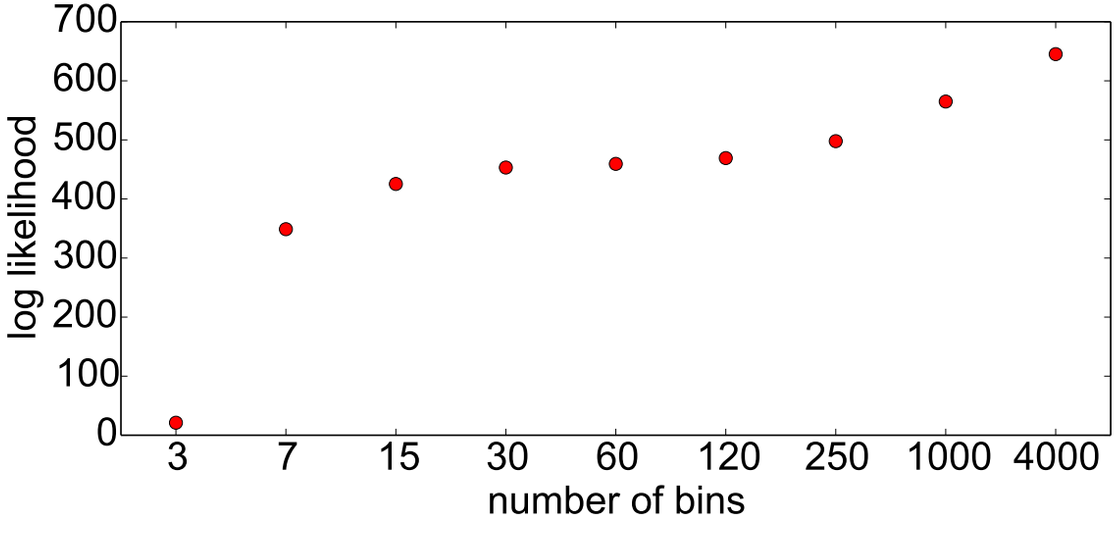
Histogram: Choosing the number of bins B (1)

Let us again employ the ML approach, this time for choosing the number of bins B:



$$L = \sum_{j=1}^{B} N_j \log h_j,$$

with $h_j = B\frac{N_j}{N}$

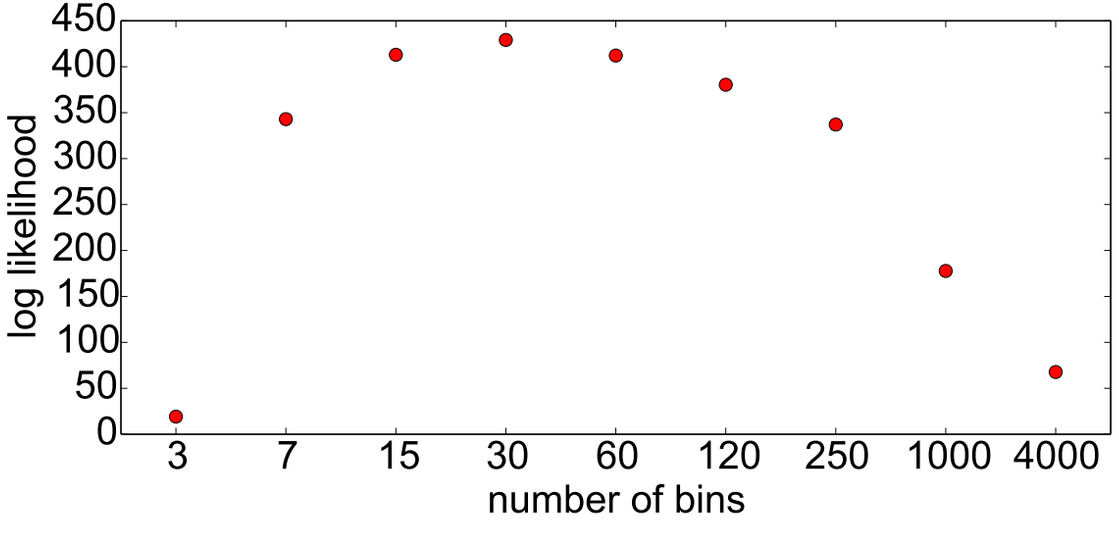


$$L = \sum_{j=1}^{B} N_j \log h_j,$$

with $h_j = B\frac{N_j+1}{N+B}$

Histogram: Choosing the number of bins B, cross-validation

The problem is that the log-likelihood L is computed using the same data used for fitting the model (computing h_i's). This is a similar concept to training a classifier on certain data and testing on the same data, which is prone to over-fitting and poor generalization.
Let us compute the log likelihood using the following procedure: remove a given point from the dataset for computing h_i's and evaluate its contribution to the log-likelihood. Do this for all the points. If we start from e.g. $h_j = B\frac{N_j+1}{N+B}$, the modified estimation of h_j (omitting the point in question) will become $h_j = B\frac{N_j}{N-1+B}$. This leads to the following result:



$$L = \sum_{j=1}^{B} N_j \log h_j,$$

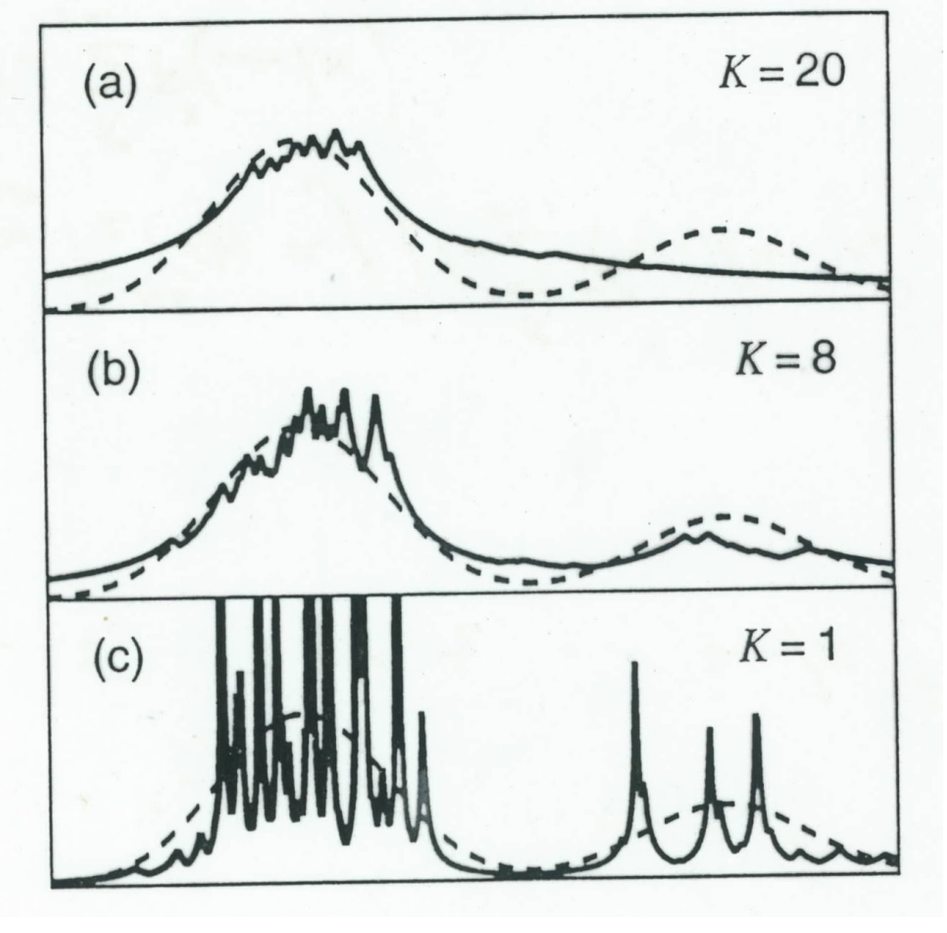
with $h_j = B\frac{N_j}{N+B-1}$

This approach is related to cross-validation technique for choosing parameters of a classifier.

K-Nearest Neighbor Approach to Density Estimation

Find K neighbors, density estimate is $p \sim 1/V$ where V is the volume of minimum cell in which K neighbors are located.

Example:



K-Nearest Neighbor Approach to Classification

Outline:

- Definition
- Properties
- Asymptotic error of NN classifier
- Error reduction by edit operation on the training class
- Fast NN search

K-NN Classification Definition

Assumption:

- Training set $\mathcal{T} = \{(x_1, k_1), (x_2, k_2), ..., (x_N, k_N)\}$. There are R classes (letter K is reserved for KNN in this lecture)
- A distance function $d : X \times X \mapsto \mathbb{R}_0^+$

Algorithm:

1. Given x, find K points $S = \{(x'_1, k'_1), (x'_2, k'_2), ..., (x'_K, k'_K)\}$ from the training set $\mathcal{T}$ which are closest to x in the metric d:

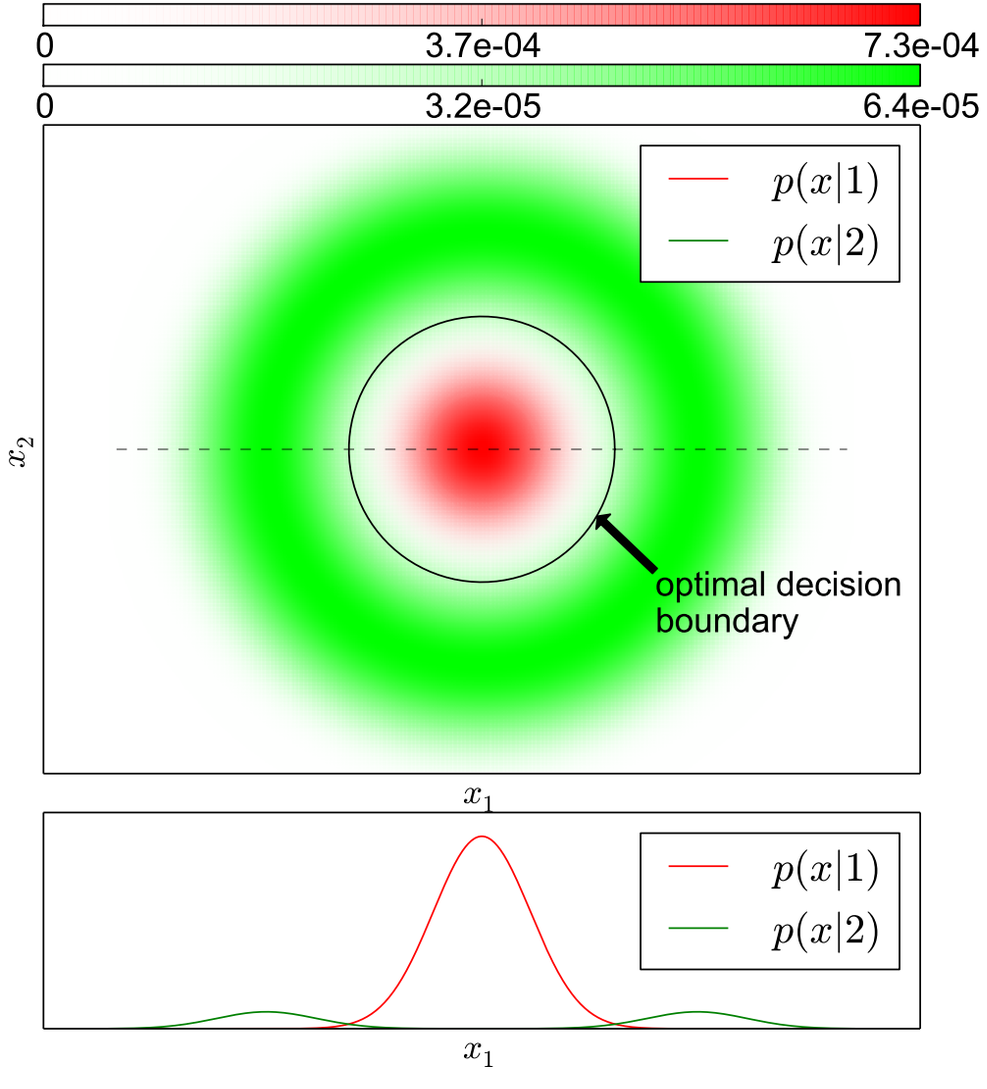
$$S = \{(x'_1, k'_1), (x'_2, k'_2), ..., (x'_K, k'_K)\} \equiv \{(x_{r_1}, k_{r_1}), (x_{r_2}, k_{r_2}), ..., (x_{r_K}, k_{r_K})\} \quad (11)$$

$$r_i\text{: the rank of } (x_i, k_i) \in \mathcal{T} \text{ as given by the ordering } d(x, x_i) \quad (12)$$

2. Classify x to the class k which has majority in S:

$$k = \underset{l \in R}{\text{argmax}} \sum_{i=1}^{K} [\![k'_i = l]\!] \qquad (x'_i, k'_i) \in S \quad (13)$$

K-NN Example (1)



the profile of the distributions along the shown line

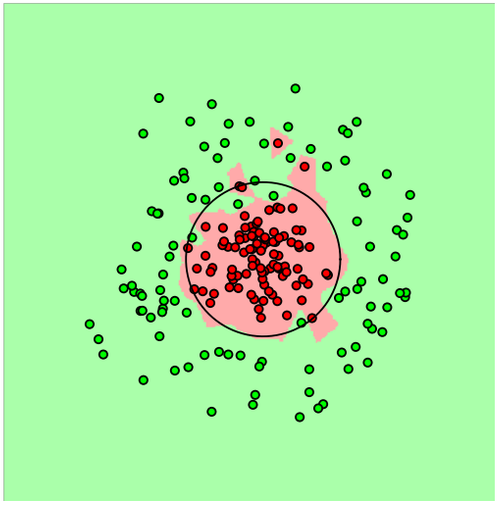
Consider the two distributions shown. They are assumed to have the same priors,

$$p(1) = p(2) = 0.5.$$

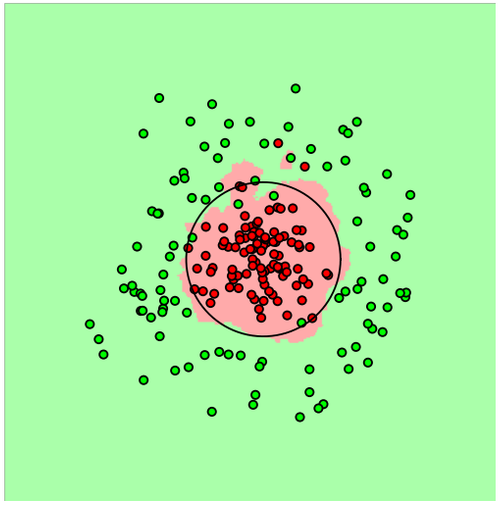
The Bayesian optimal decision boundary is shown by the black circle.

K-NN Example (2)

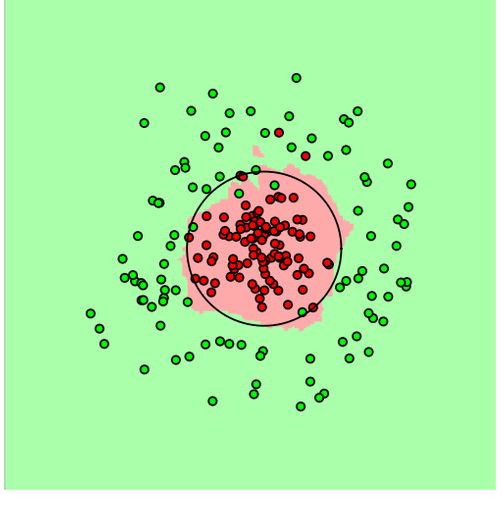
NN classification, K = 1



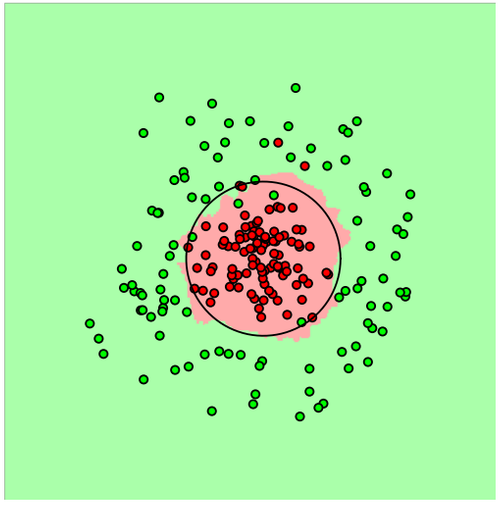
NN classification, K = 3



NN classification, K = 5



NN classification, K = 7



($N = 100$ samples from each distribution)

K-NN Properties

- Trivial implementation ($\rightarrow$ good baseline method)
- 1-NN: Bayes error ϵ_B is the lower bound on error of classification ϵ_{NN} (in the asymptotic case $N \rightarrow \infty$.) Higher bounds can also be constructed, e.g. $\epsilon_{NN} \leq 2\epsilon_B$
- Slow when implemented naively, but can be sped up (Voronoi, k-D trees)
- High computer memory requirements (but training set can be edited and its cardinality decreased)
- How to construct the metric d? (problem of scales in different axes)

K-NN : Speeding Up the Classification

- Sophisticated algorithms for NN search:
  - Classical problem in Comp. Geometry
  - k-D trees
- Removing the samples from the training class $\mathcal{T}$ which do not change the result of classification
  - Exactly: using Voronoi diagram
  - Approximately: E.g. use Gabriel graph instead of Voronoi
  - Condensation algorithm: iterative, also approximate.

Condensation Algorithm

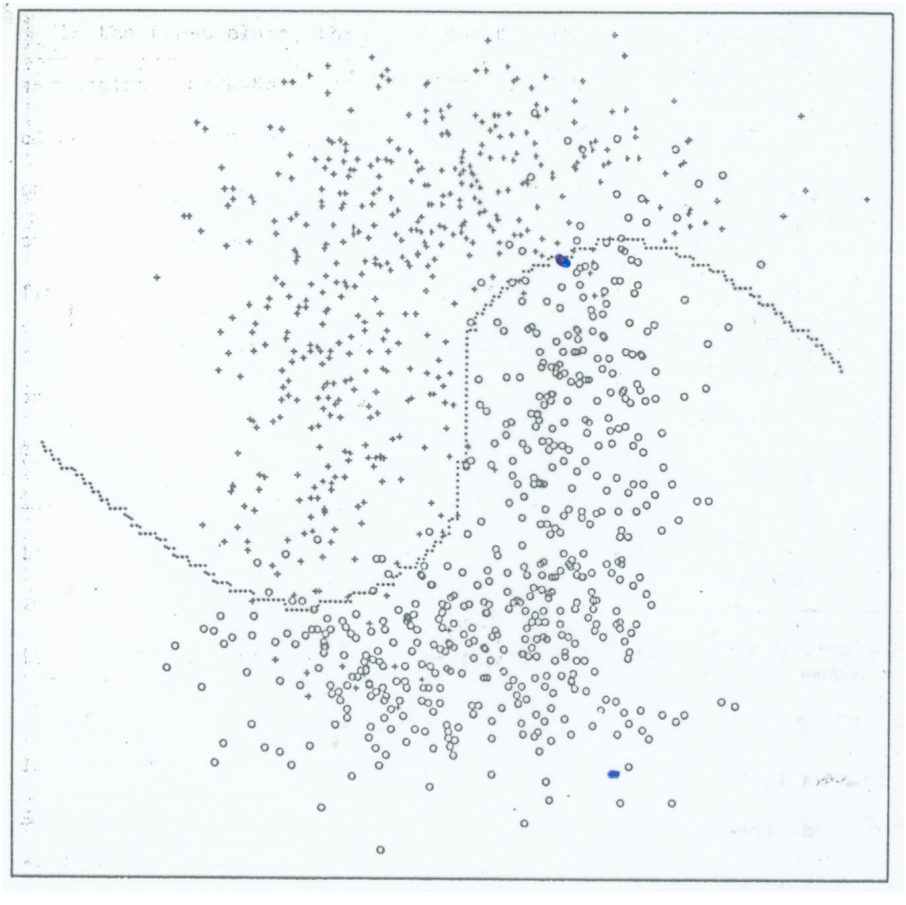
Input: The training set $\mathcal{T}$.

Algorithm

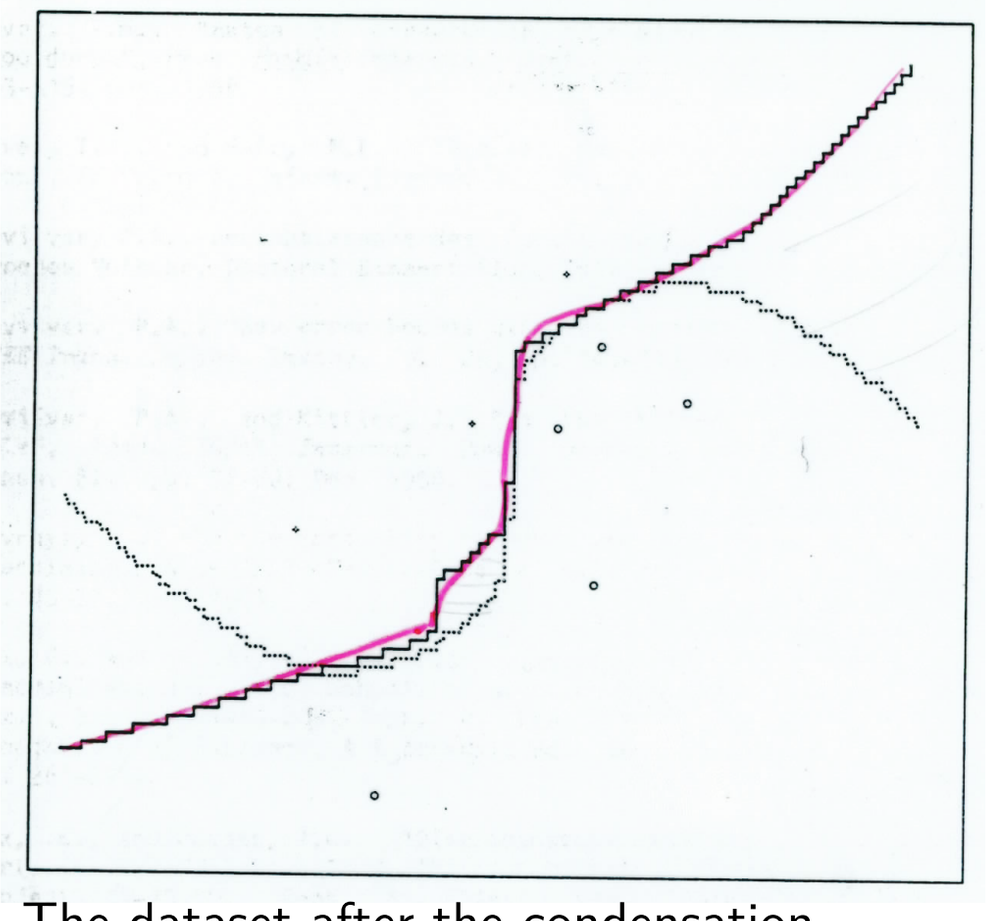
1. Create two lists, A and B. Insert a randomly selected sample from $\mathcal{T}$ to A. Insert the rest of the training samples to B.
2. Classify samples from B using 1NN with training set A. If an $x \in B$ is mis-classified, move it from B to A.
3. If a move has been triggered in Step 2., goto Step 2.

Output: A (the condensed training set for 1NN classification)

Condensation Algorithm, Example



The training dataset



The dataset after the condensation.
Shown with the new decision boundary.

1-NN Classification Error

Recall that a classification error $\bar{\epsilon}$ for strategy $q\colon X \to R$ is computed as

$$\bar{\epsilon} = \int \sum_{k:q(x)\neq k} p(x,k)\mathrm{d}x = \int \underbrace{\sum_{k:q(x)\neq k} p(k|x)}_{\epsilon(x)} p(x)\mathrm{d}x = \int \epsilon(x)p(x)\mathrm{d}x\,. \tag{14}$$

We know that the Bayesian strategy q_B decides for the highest posterior probability $q(x) = \mathrm{argmax}_k\, p(k|x)$, thus the partial error $\epsilon_B(x)$ for a given x is

$$\epsilon_B(x) = 1 - \max_k p(k|x)\,. \tag{15}$$

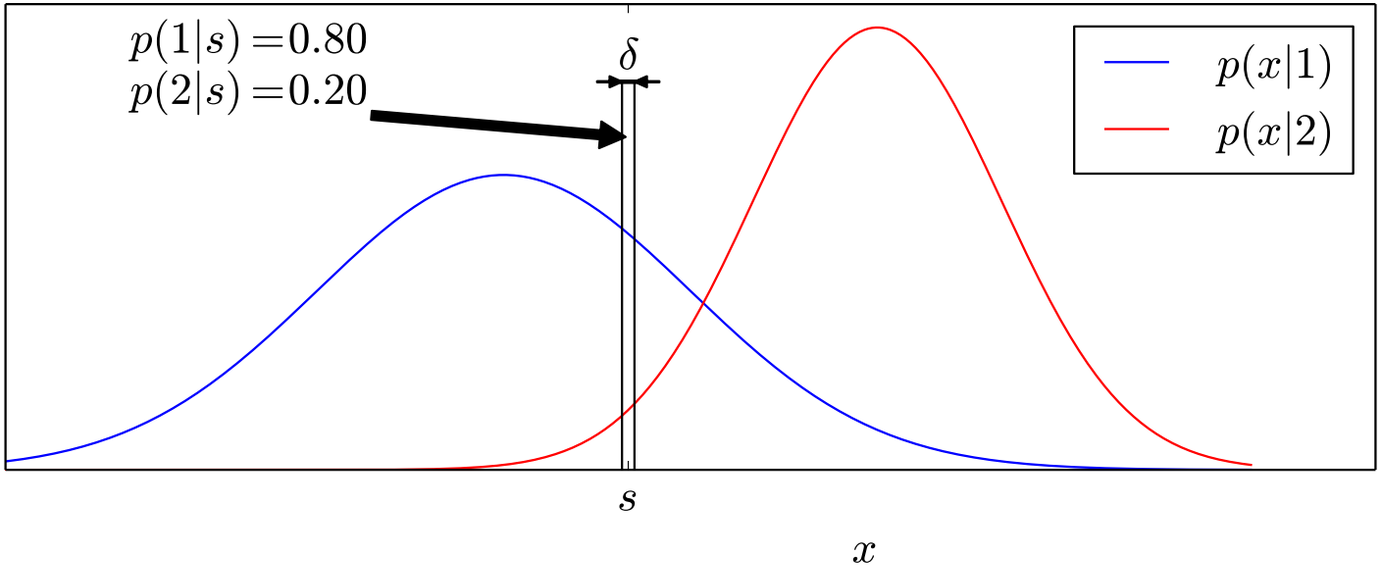
Assume the asymptotic case. We will show that the following bounds hold for the partial error $\epsilon_{NN}(x)$ and classification error $\bar{\epsilon}_{NN}$ in the 1-NN classification,

$$\epsilon_B(x) \leq \epsilon_{NN}(x) \leq 2\epsilon_B(x) - \tfrac{R}{R-1}\epsilon_B^2(x)\,, \tag{16}$$

$$\bar{\epsilon}_B \leq \bar{\epsilon}_{NN} \leq 2\bar{\epsilon}_B - \tfrac{R}{R-1}\bar{\epsilon}_B^2\,, \tag{17}$$

where $\bar{\epsilon}_B$ is the Bayes classification error and R is the number of classes.

1-NN Classification Error, Example (1)



Consider two distributions as shown, a small interval δ on an x-axis, and a point $s \in \delta$. Let the class priors be $p(1) = p(2) = 0.5$. Assume $\delta \to 0$ and number of samples $N \to \infty$.

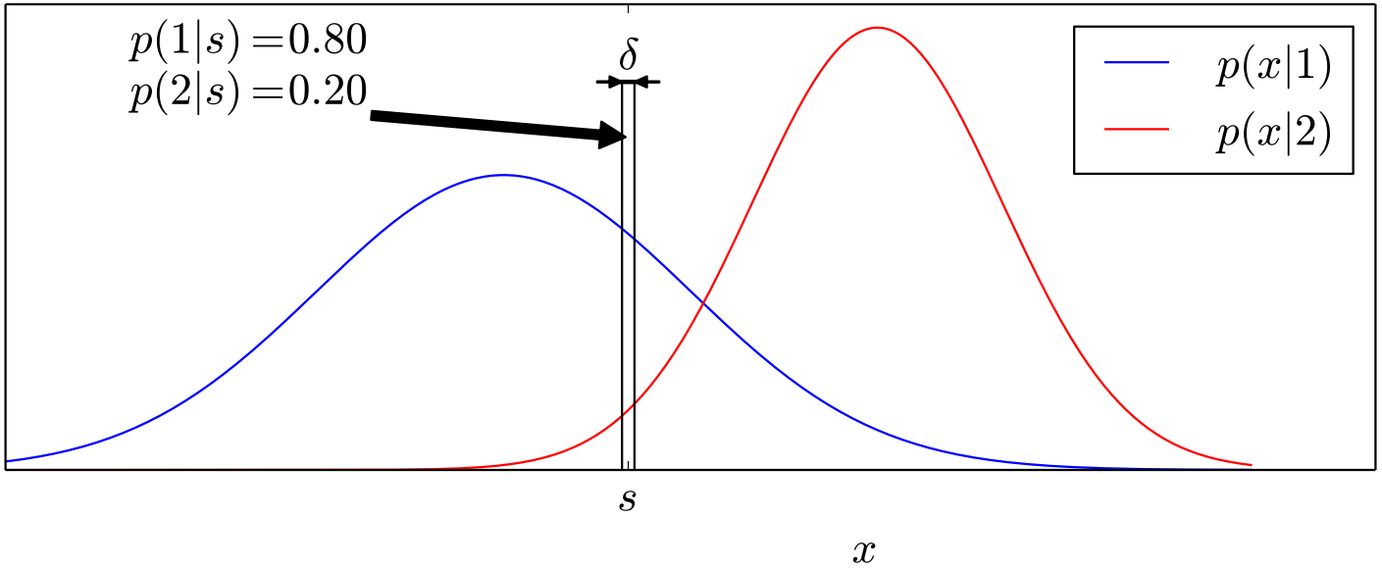
Observe the following:

$$p(1|s) = 0.8\,, \quad p(2|s) = 0.2\,, \tag{18}$$

$$p(NN = 1|s) = p(1|s) = 0.8\,, \quad p(NN = 2|s) = p(2|s) = 0.2\,, \tag{19}$$

where $p(NN = k|s)$ is the probability that the 1-NN of s is from class k ($k = 1, 2$) and thus s is classified as k.

1-NN Classification Error, Example (2)



The error $\epsilon_{NN}(s)$ at s is

$$\epsilon_{NN}(s) = p(1|s)p(NN = 2|s) + p(2|s)p(NN = 1|s) \tag{20}$$

$$= 1 - p(1|s)p(NN = 1|s) - p(2|s)p(NN = 2|s) \tag{21}$$

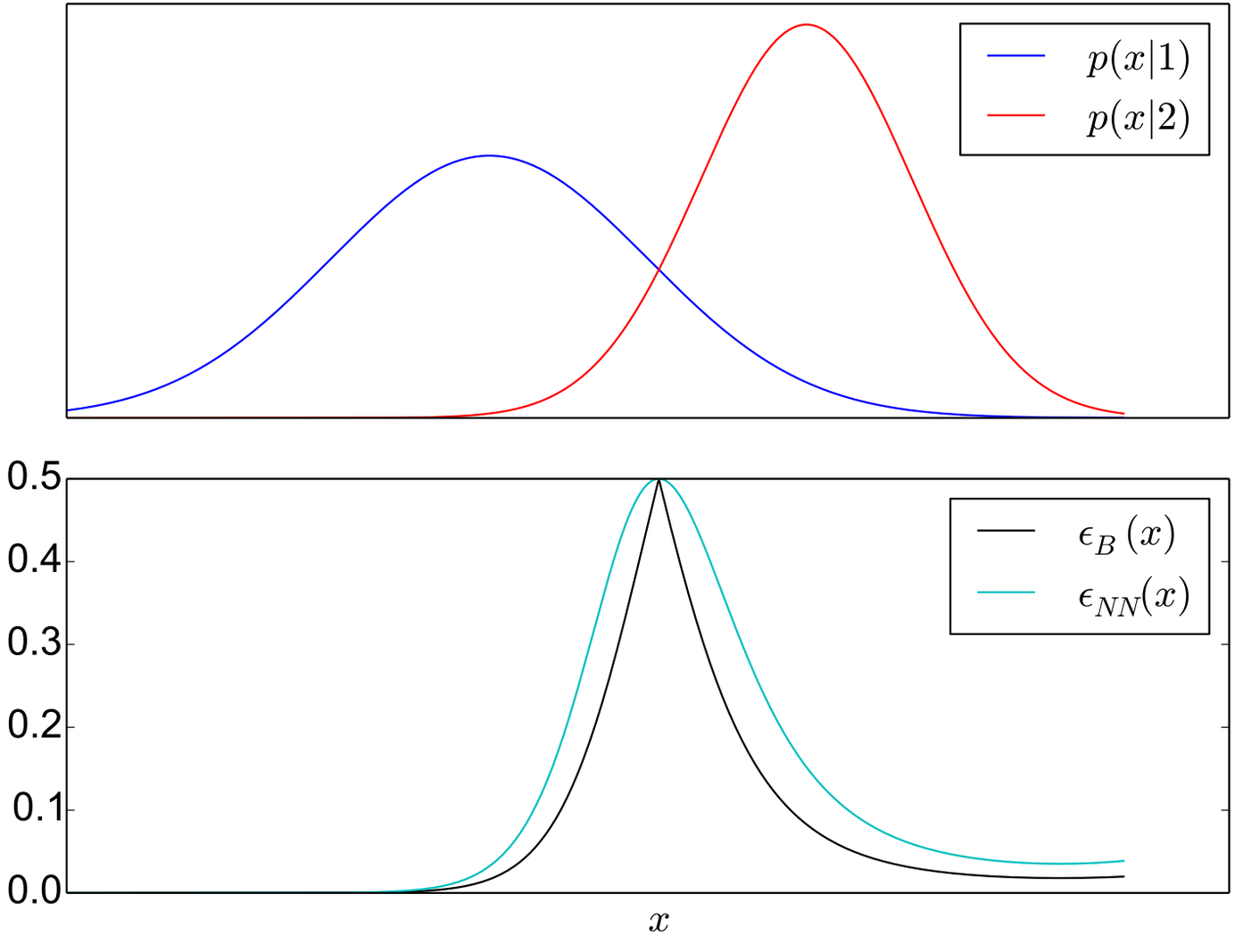
$$= 1 - p^2(1|s) - p^2(2|s)\,. \tag{22}$$

Generally, for R classes, the error will be

$$\epsilon_{NN}(s) = 1 - \sum_{k \in R} p^2(k|s)\,. \tag{23}$$

1-NN Classification Error, Example (3)

The two distributions and the partial errors
(the Bayesian error $\epsilon_B(x)$ and the 1-NN error $\epsilon_{NN}(x)$)



1-NN Classification Error Bounds (1)

Let us now return to the inequalities and prove them:

$$\epsilon_B(x) \leq \epsilon_{NN}(x) \leq 2\epsilon_B(x) - \frac{R}{R-1}\epsilon_B^2(x)\,, \tag{24}$$

The **first** inequality follows from the fact that Bayes strategies are optimal.

To prove the **second** inequality, let $P(x)$ denote the maximum posterior for x:

$$P(x) = \max_k p(k|x) \tag{25}$$

$$\Rightarrow \quad \epsilon_B(x) = 1 - P(x)\,. \tag{26}$$

Let us rewrite the partial error $\epsilon_{NN}(x)$ using the Bayesian entities $P(x)$ and $q(x)$:

$$\epsilon_{NN}(x) = 1 - \sum_{k \in R} p^2(k|x) = 1 - P^2(x) - \sum_{k \neq q(x)} p^2(k|x)\,. \tag{27}$$

We know that $p(q(x)|x) = P(x)$, but the remaining posteriors can be arbitrary. Let us consider the worst case. i.e. set $p(k|x)$ for $k \neq q(x)$ such that Eq. (27) is maximized. This will provide the higher bound.

1-NN Classification Error Bounds (2)

There are the following constraints on $p(k|x)$ $(k \neq q(x))$:

$$\sum_{k \neq q(x)} p(k|x) + P(x) = 1 \qquad \text{(posteriors sum to 1)} \tag{28}$$

$$\sum_{k \neq q(x)} p^2(k|x) \to \min \tag{29}$$

It is easy to show that this optimization problem is solved by setting all the posteriors to the same number. Thus,

$$p(k|x) = \frac{1 - P(x)}{R - 1} = \frac{\epsilon_B(x)}{R - 1} \qquad (k \neq q(x)) \tag{30}$$

The higher bound can then be rewritten in terms of the Bayes partial error $\epsilon_B(x) = 1 - P(x)$:

$$\epsilon_{NN}(x) \leq 1 - P^2(x) - \sum_{k \neq q(x)} p^2(k|x) = 1 - (1 - \epsilon_B(x))^2 - (R - 1)\frac{\epsilon_B^2(x)}{(R - 1)^2}\,. \tag{31}$$

1-NN Classification Error Bounds (3)

$$\epsilon_{NN}(x) \leq 1 - P^2(x) - \sum_{k \neq q(x)} p^2(k|x) = 1 - (1 - \epsilon_B(x))^2 - \frac{\epsilon_B^2(x)}{R-1}\,. \tag{32}$$

After expanding this, we get

$$\epsilon_{NN}(x) \leq 1 - (1 - \epsilon_B(x))^2 - \frac{\epsilon_B^2(x)}{(R-1)} \tag{33}$$

$$= 1 - 1 + 2\epsilon_B(x) - \epsilon_B^2(x) - \epsilon_B^2(x)\frac{R}{R-1} \tag{34}$$

$$= \quad 2\epsilon_B(x) - \epsilon_B^2(x)\tfrac{R}{R-1} \tag{35}$$

Note that for $R = 2$, the bound is tight because using $\epsilon_B(x) = 1 - P(x)$ in Eq. (32) gives

$$\epsilon_{NN}(x) \leq 1 - P^2(x) - \frac{(1 - P(x))^2}{1} = \epsilon_{NN}(x)\,. \tag{36}$$

1-NN Classification Error Bounds (4)

The inequality for the local errors has been proven:

$$\epsilon_{NN}(x) \leq 2\epsilon_B(x) - \epsilon_B^2(x)\frac{R}{R-1} \tag{37}$$

Is there a similar higher bound for the classification error $\bar{\epsilon}_{NN} = \int \epsilon_{NN}(x)p(x)\mathrm{d}x$, based on the Bayes error $\bar{\epsilon}_B = \int \epsilon_B(x)p(x)\mathrm{d}x$?

Multiplying Eq. (38) by $p(x)$, and integrating, gives

$$\bar{\epsilon}_{NN} \leq 2\bar{\epsilon}_B(x) - \frac{R}{R-1}\int \epsilon_B^2(x)p(x)\mathrm{d}x \tag{38}$$

Let us use the known identity (where $E(\cdot)$ is the expectation operator)

$$\mathrm{var}(x) = E\left(x^2\right) - E^2(x) \qquad (\geq 0) \tag{39}$$

Thus, $\int \epsilon_B^2(x)p(x)\mathrm{d}x \geq \left(\int \epsilon_B(x)p(x)\mathrm{d}x\right)^2$, and

$$\bar{\epsilon}_{NN} \leq 2\bar{\epsilon}_B(x) - \frac{R}{R-1}\int \epsilon_B^2(x)p(x)\mathrm{d}x \leq 2\bar{\epsilon}_B(x) - \frac{R}{R-1}\bar{\epsilon}_B^2 \ . \tag{40}$$

K-NN Classification Error Bound

It can be shown that for K-NN, the following inequality holds:

$$\bar{\epsilon}_{KNN} \leq \bar{\epsilon}_B + \bar{\epsilon}_{1NN}/\sqrt{K \text{ const}} \tag{41}$$

Edit algorithm

The primary goal of this method is to reduce the classification error (not the speed-up of classification.)

Input: The training set $\mathcal{T}$.

Algorithm

1. Partition $\mathcal{T}$ to two sets, A and B ($\mathcal{T} = A \cup B$, $A \cap B = \emptyset$.)
2. Classify samples in B using **K**NN with training set A. Remove all samples from B which have been mis-classified.

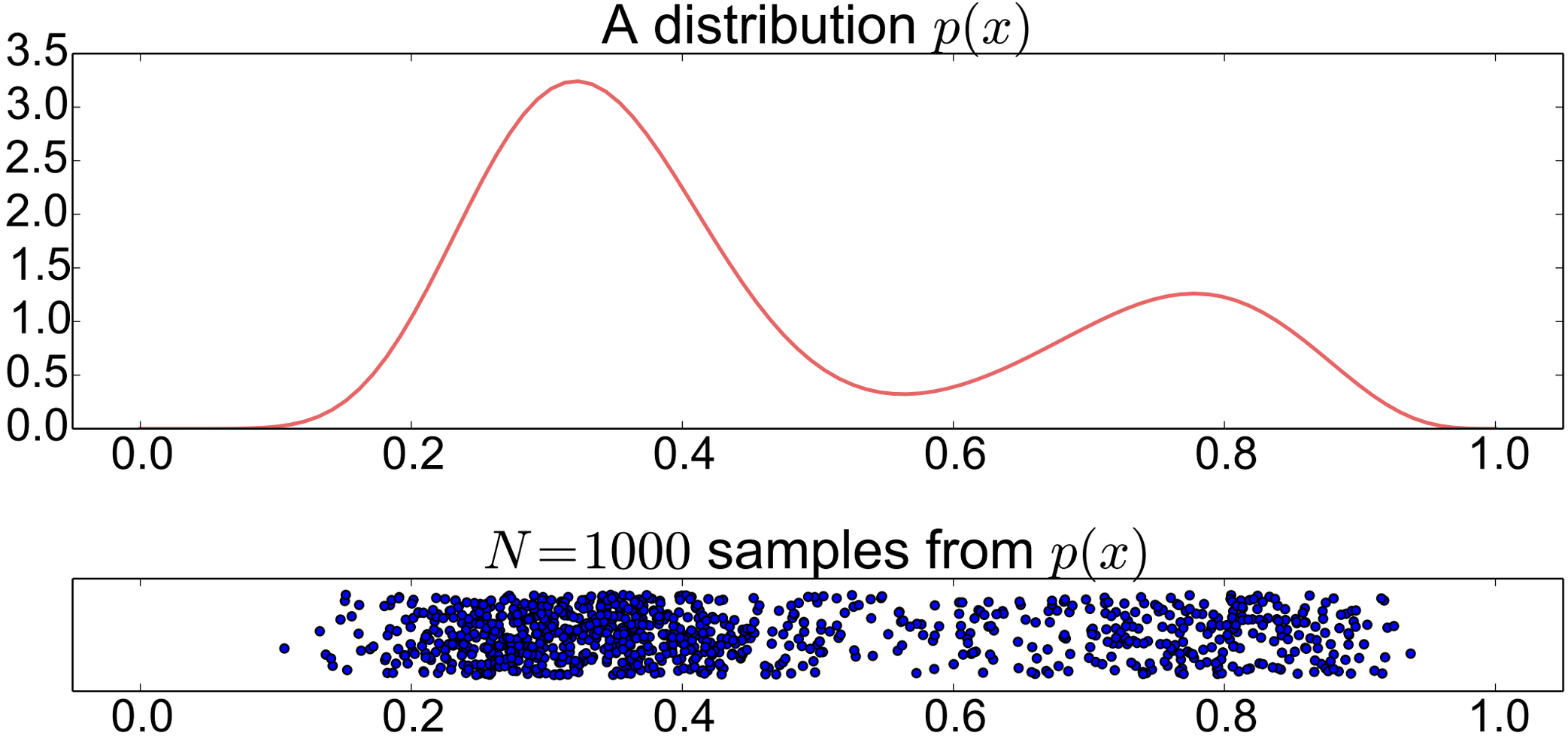
Output: B the training set for **1**NN classification.

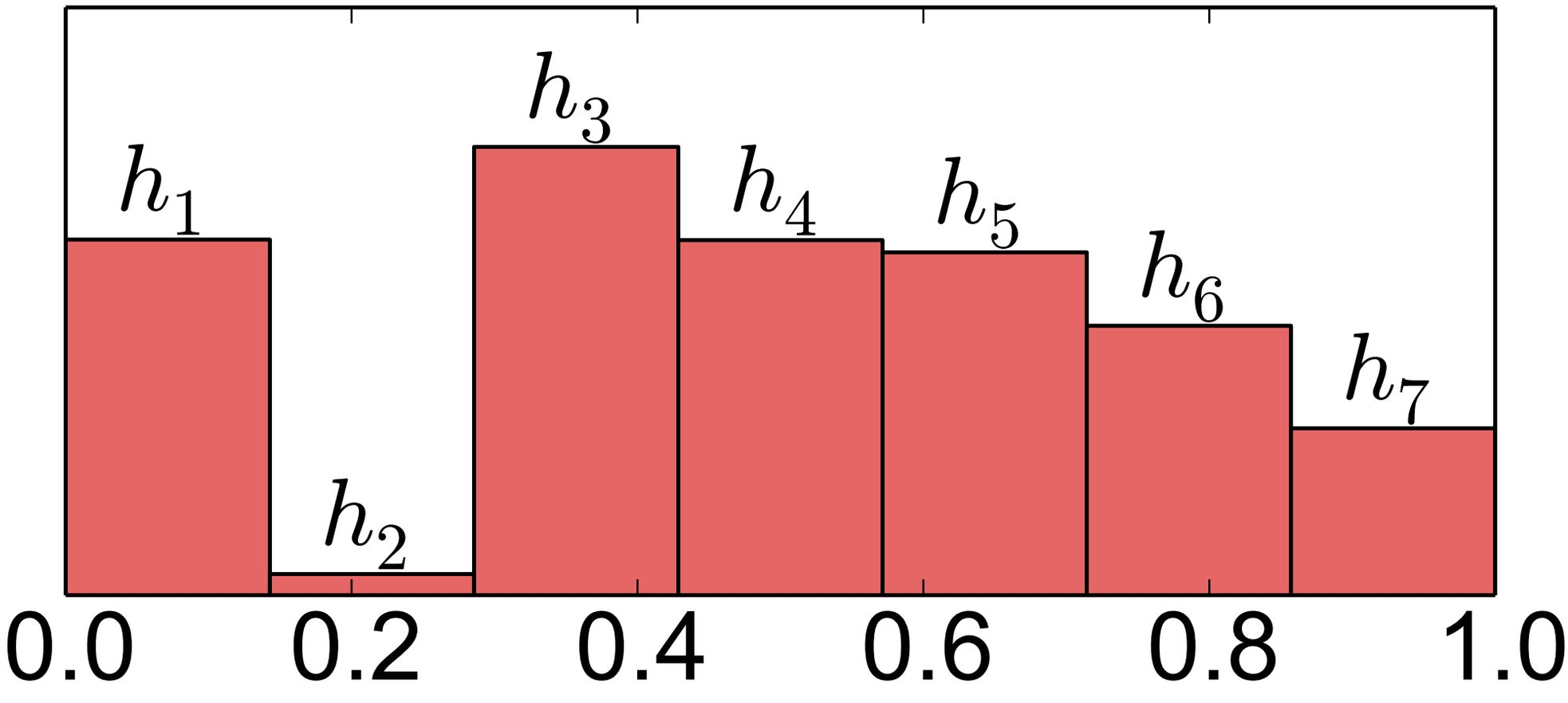
Asymptotic property:

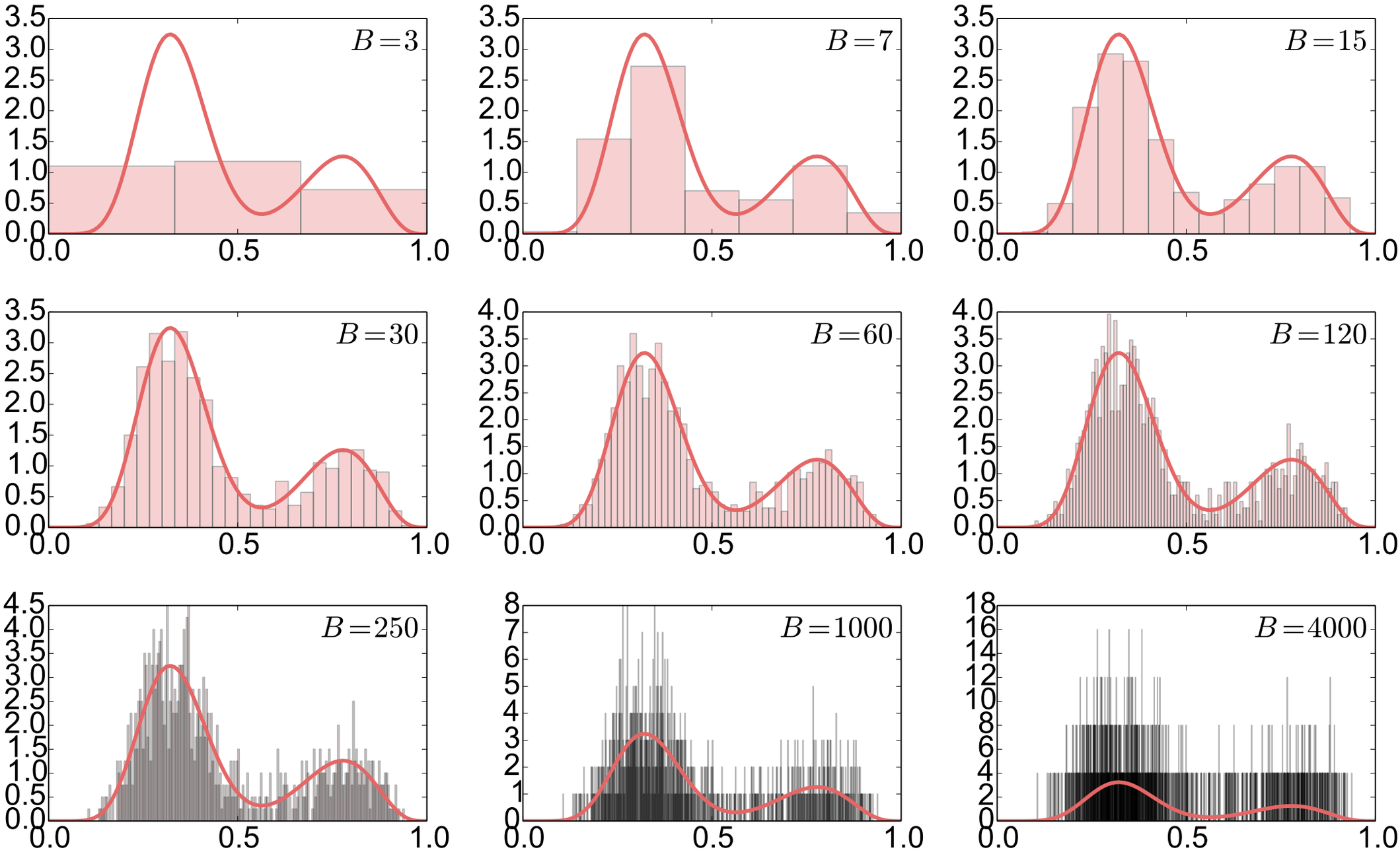
$$\bar{\epsilon}_{edit} = \bar{\epsilon}_B \frac{1 - \bar{\epsilon}_B}{1 - \bar{\epsilon}_{KNN}} \tag{42}$$

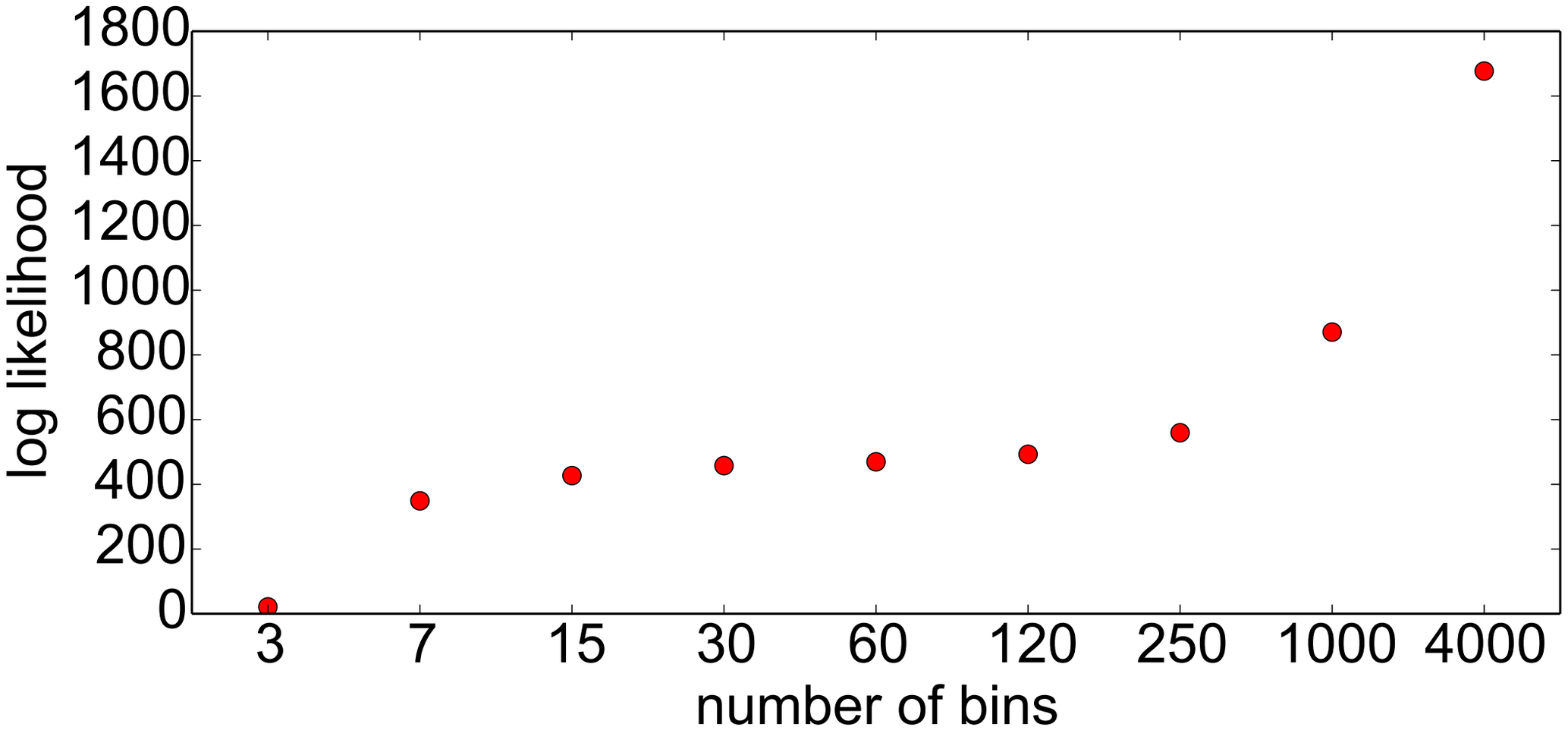
If $\bar{\epsilon}_{KNN}$ is small (e.g. 0.05) then the edited 1NN is quasi-Bayes (almost the same performance as Bayesian Classification.)

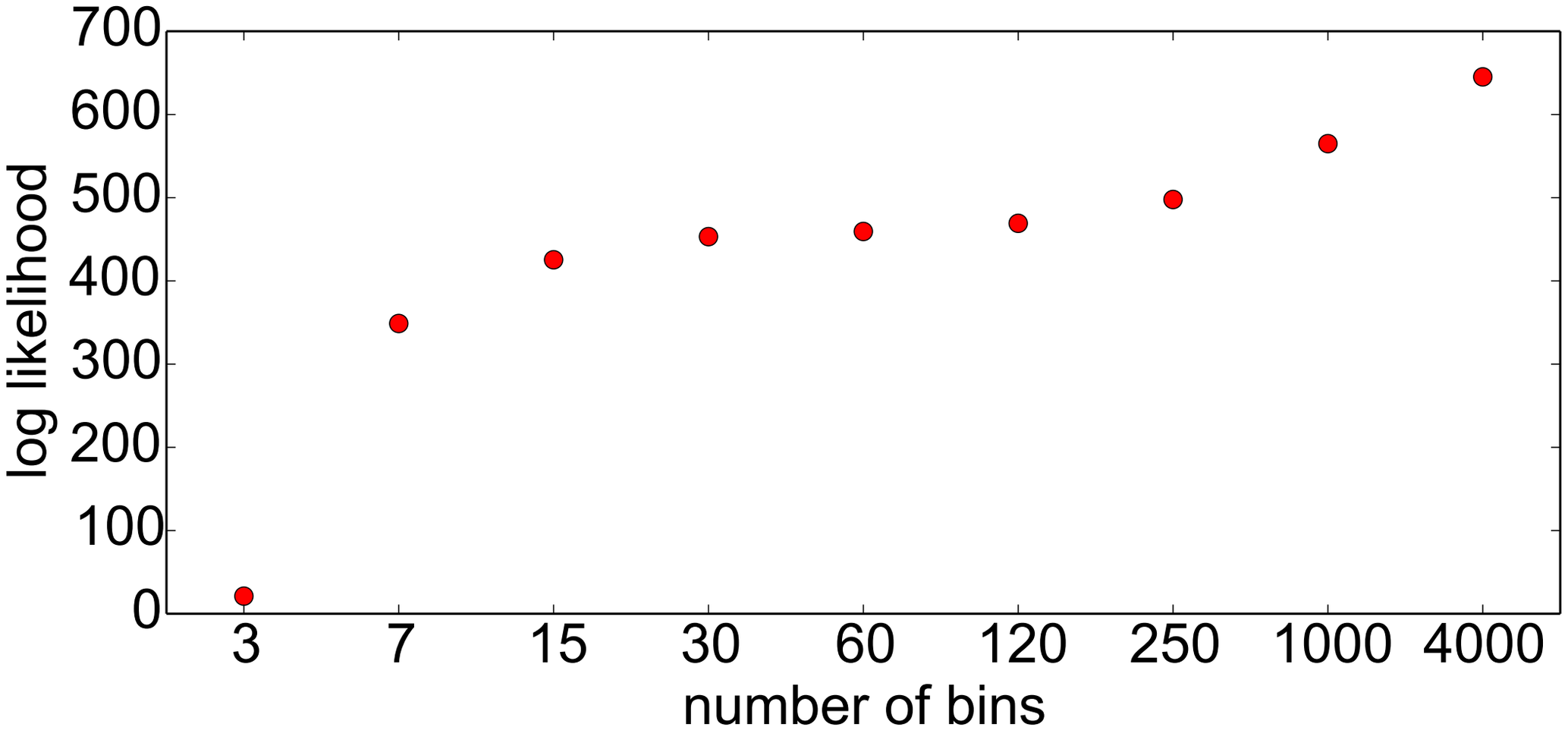

m p

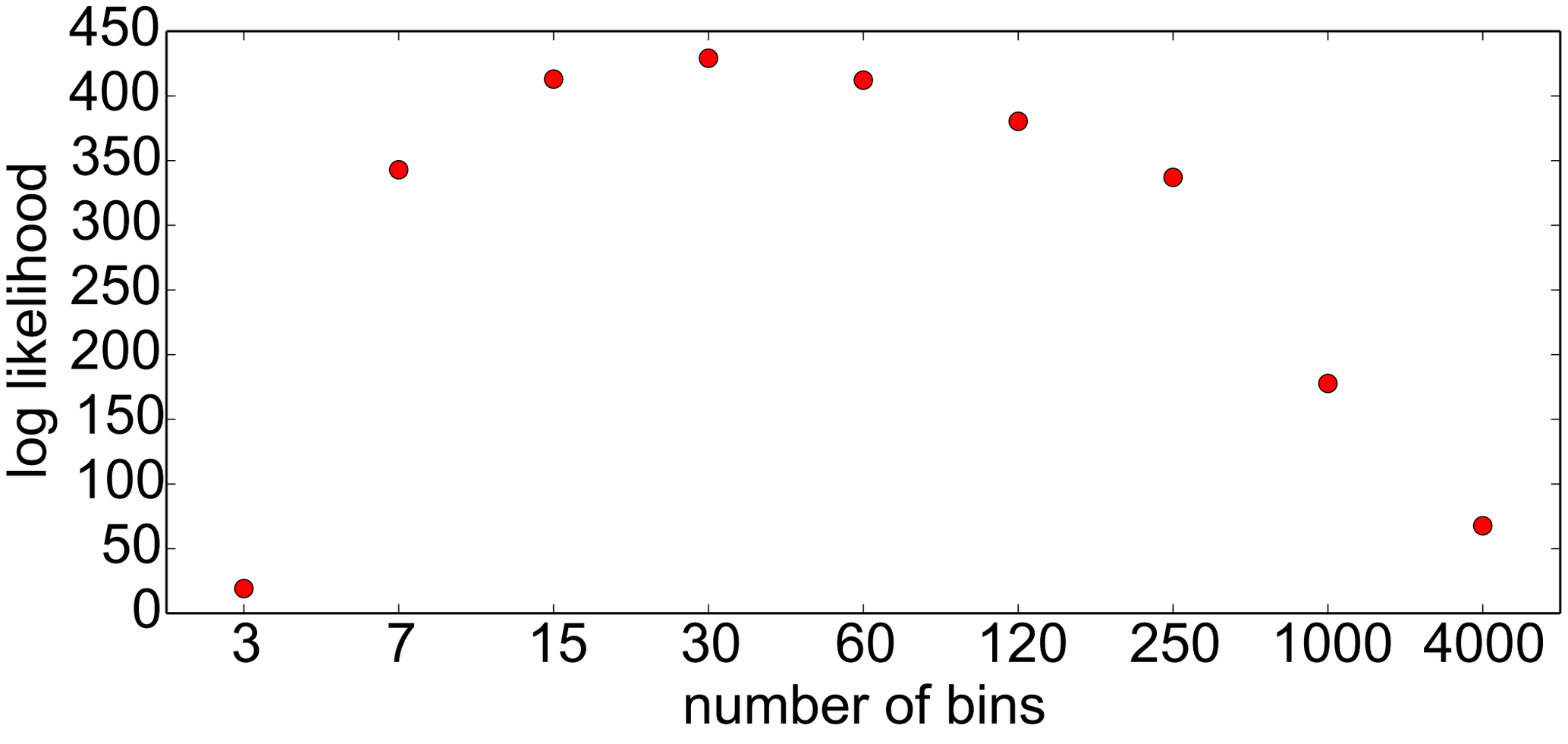

A distribution $p(x)$
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0.0
0.2
0.4
0.6
0.8
1.0
$N = 1000$ samples from $p(x)$
0.0
0.2
0.4
0.6
0.8
1.0

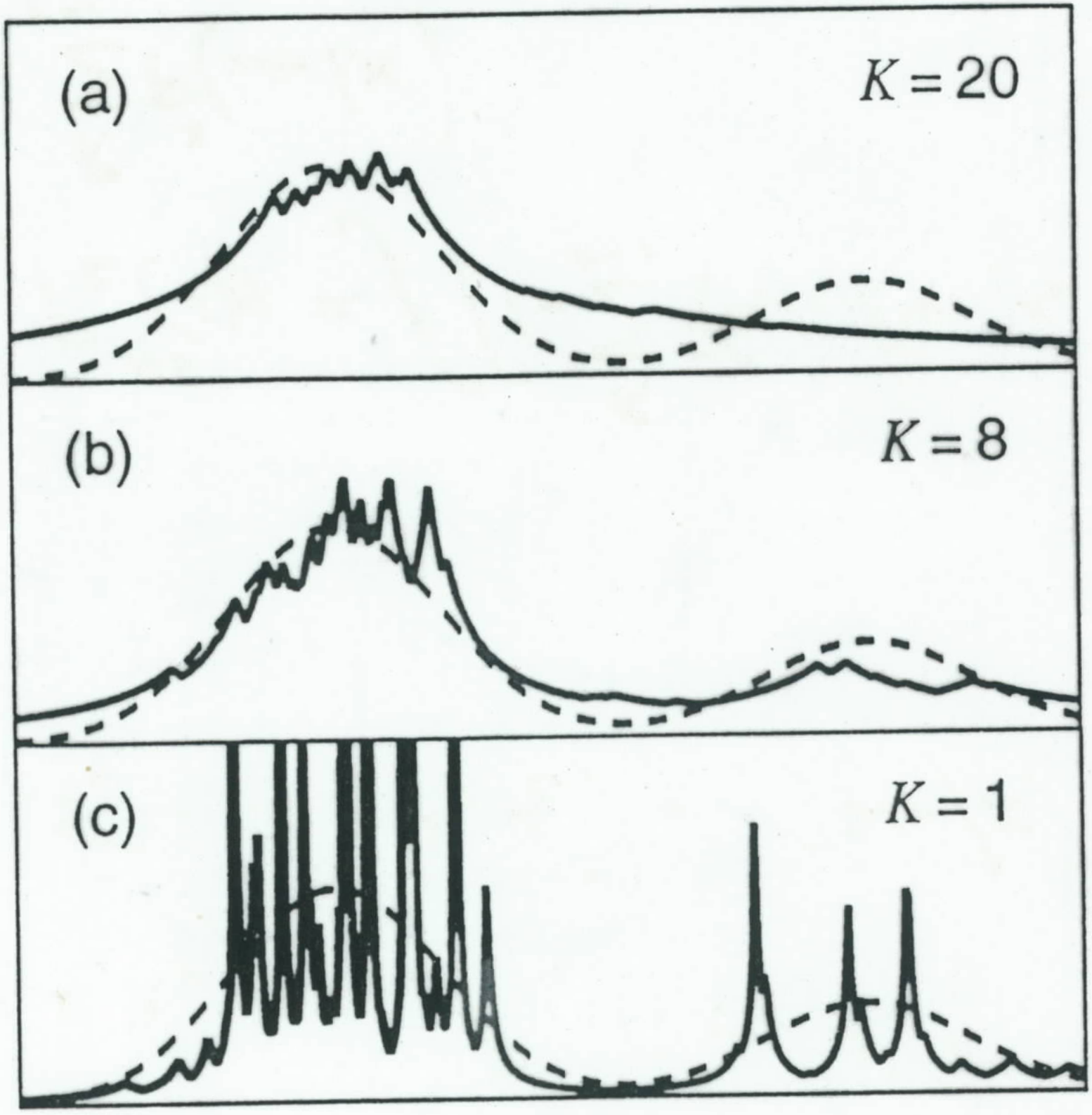

h_1
h_2
h_3
h_4
h_5
h_6
h_7
0.0
0.2
0.4
0.6
0.8
1.0

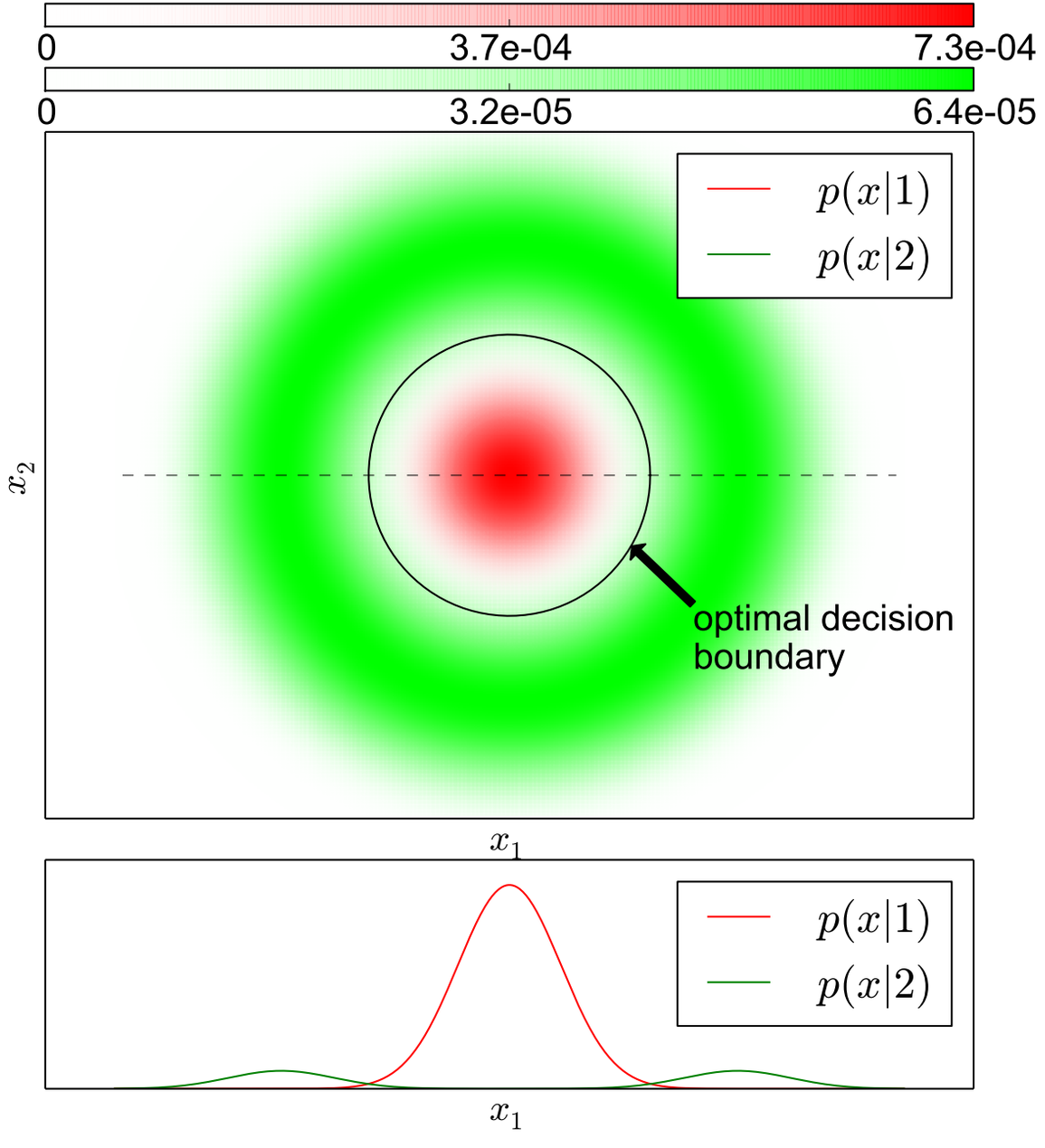

$B = 3$
$B = 7$
$B = 15$
$B = 30$
$B = 60$
$B = 120$
$B = 250$
$B = 1000$
$B = 4000$


log likelihood
1800
1600
1400
1200
1000
800
600
400
200
0
3
7
15
30
60
120
250
1000
4000
number of bins


700
600
500
400
300
200
100
0
log likelihood
3
7
15
30
60
120
250
1000
4000
number of bins

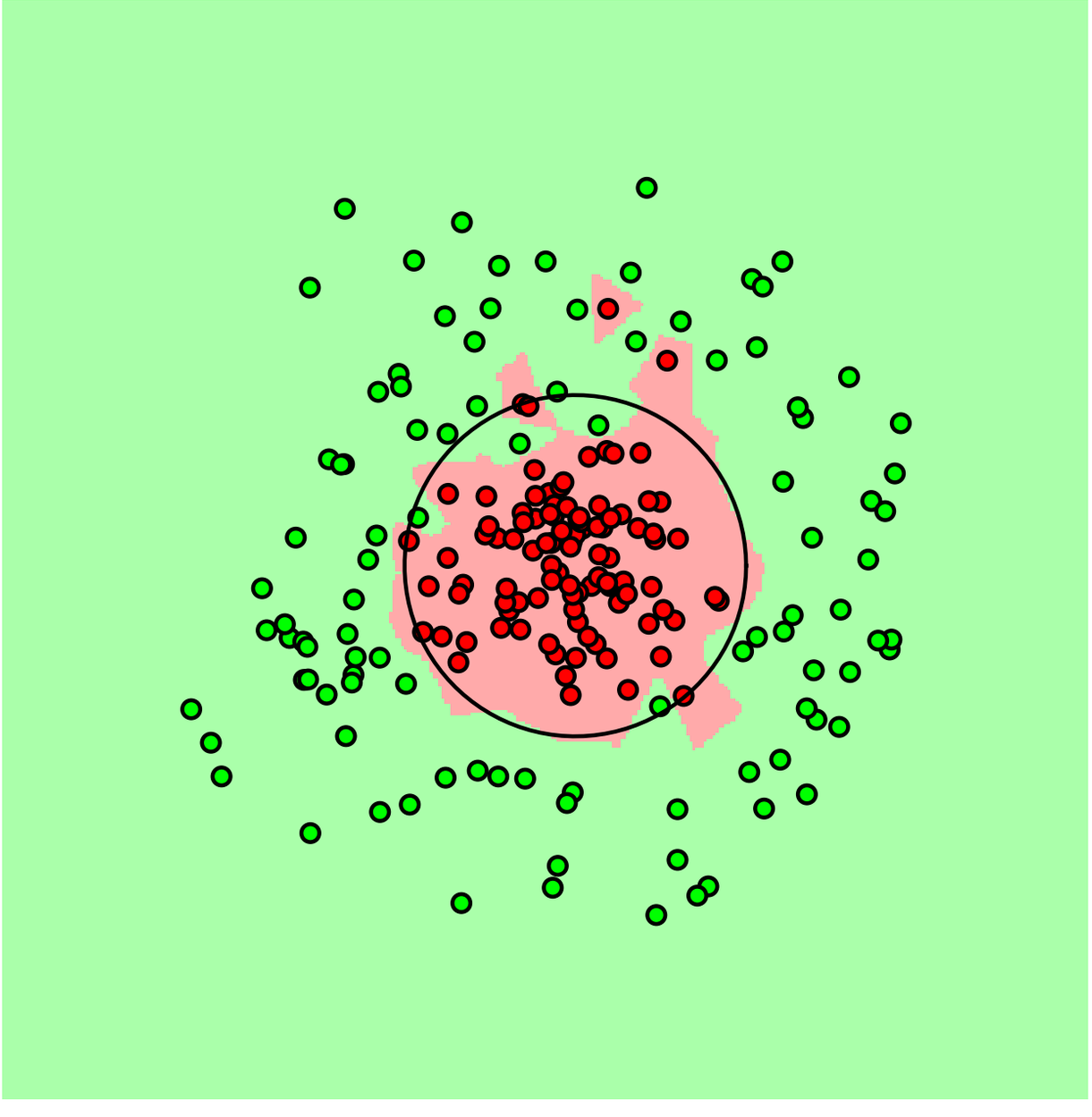

log likelihood
450
400
350
300
250
200
150
100
50
0
3
7
15
30
60
120
250
1000
4000
number of bins


(a)
K = 20
(b)
K = 8
(c)
K = 1

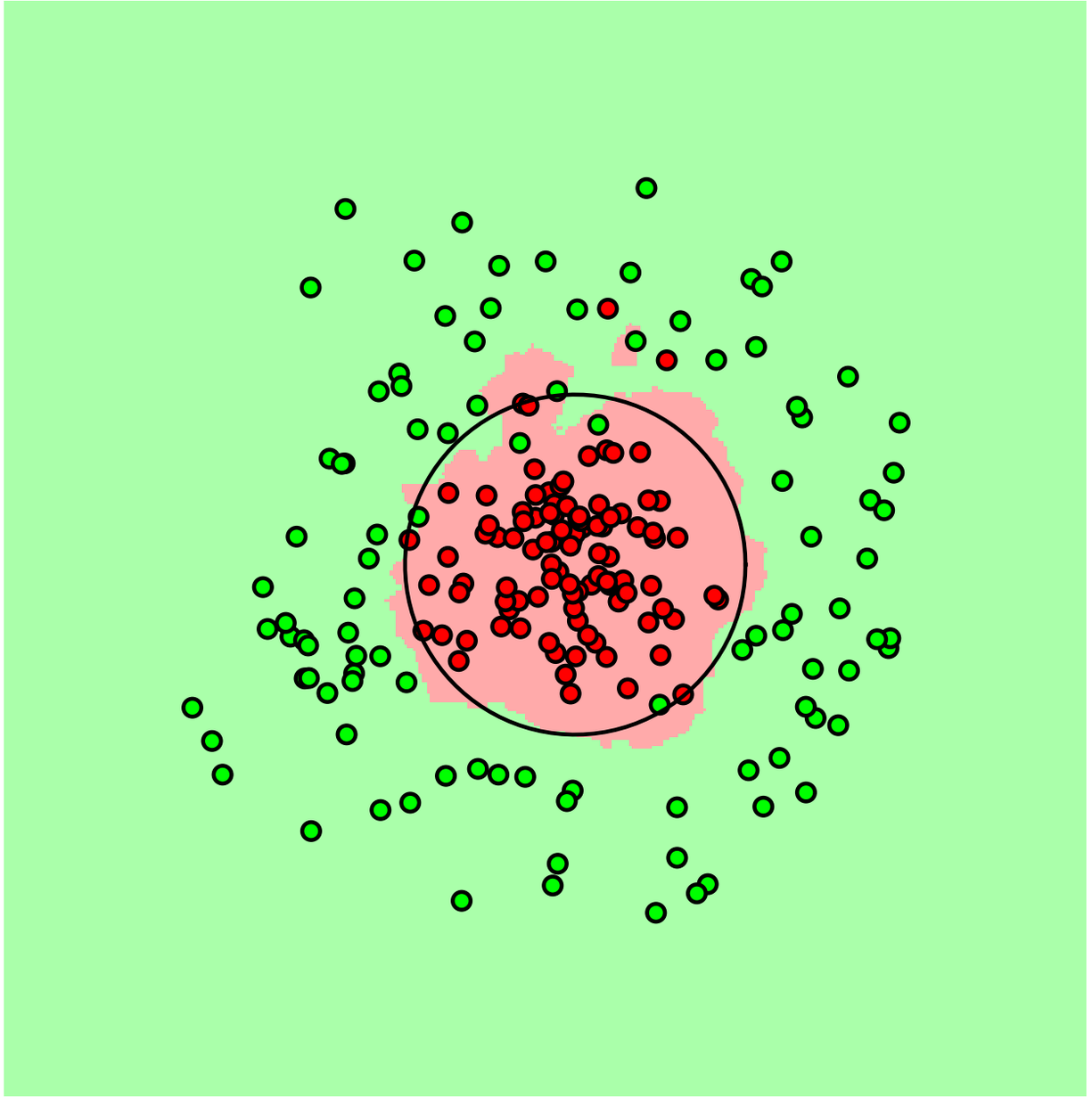


the profile of the distributions along the shown line

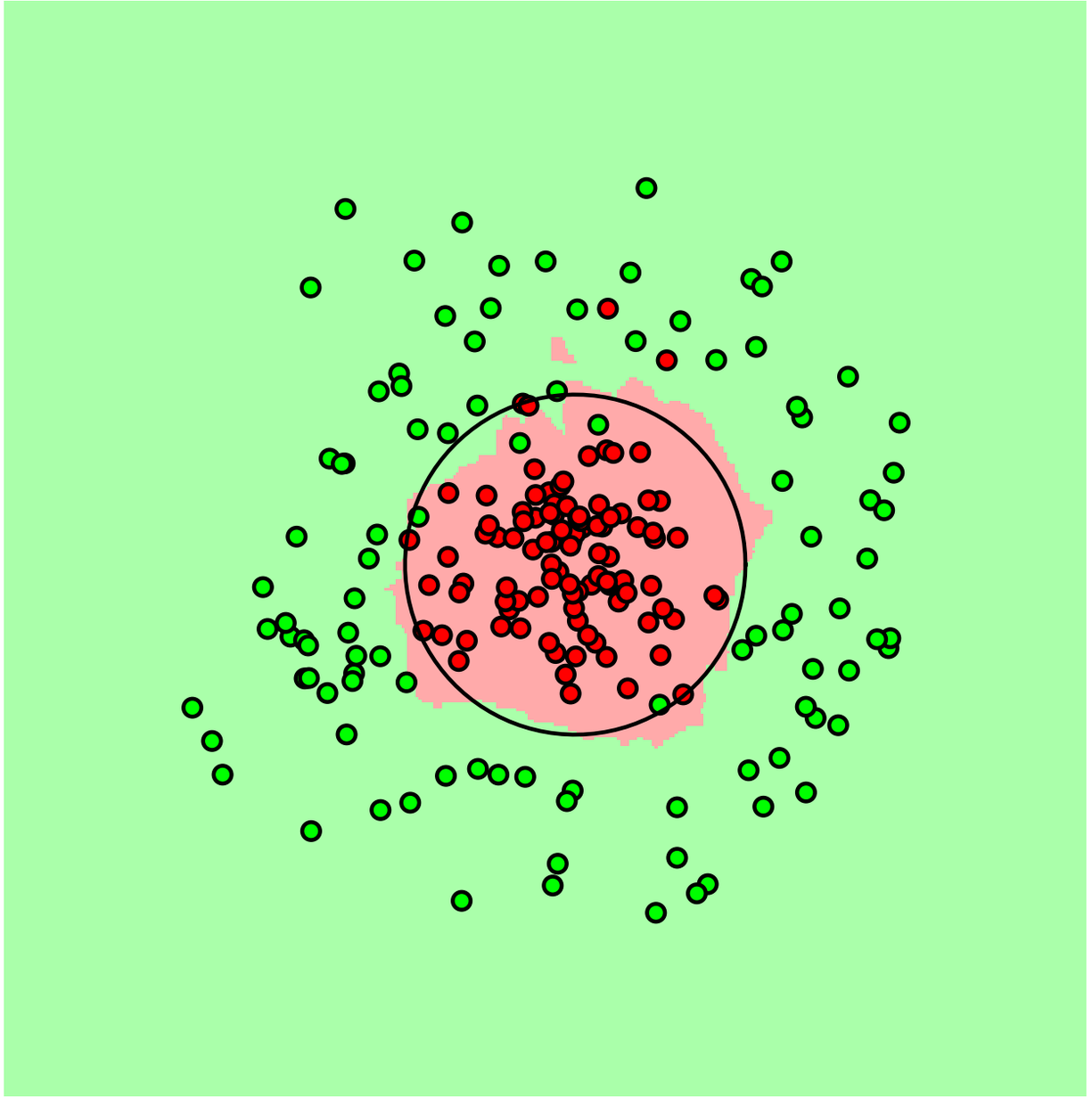
NN classification, K = 1



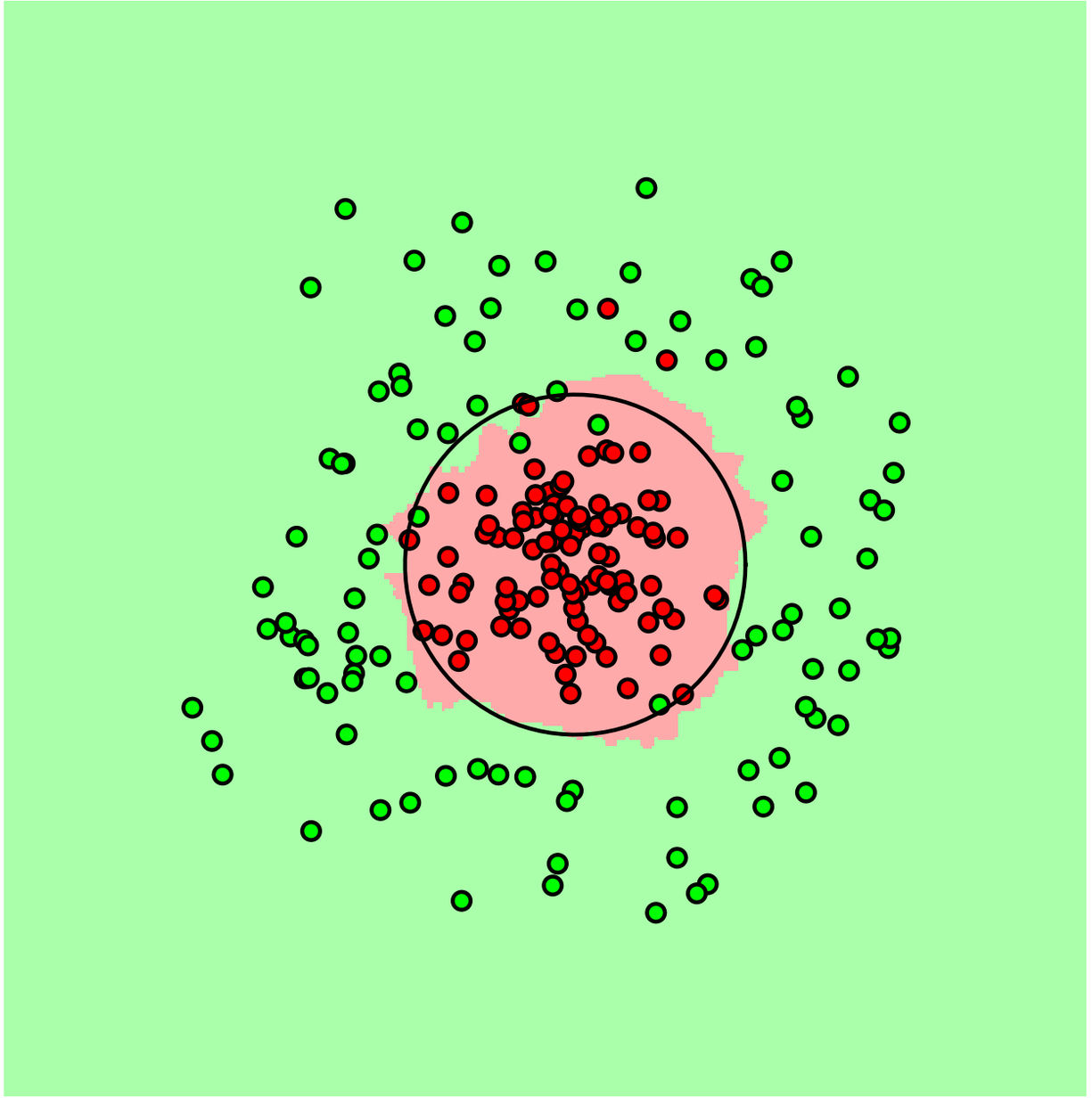
NN classification, K = 3

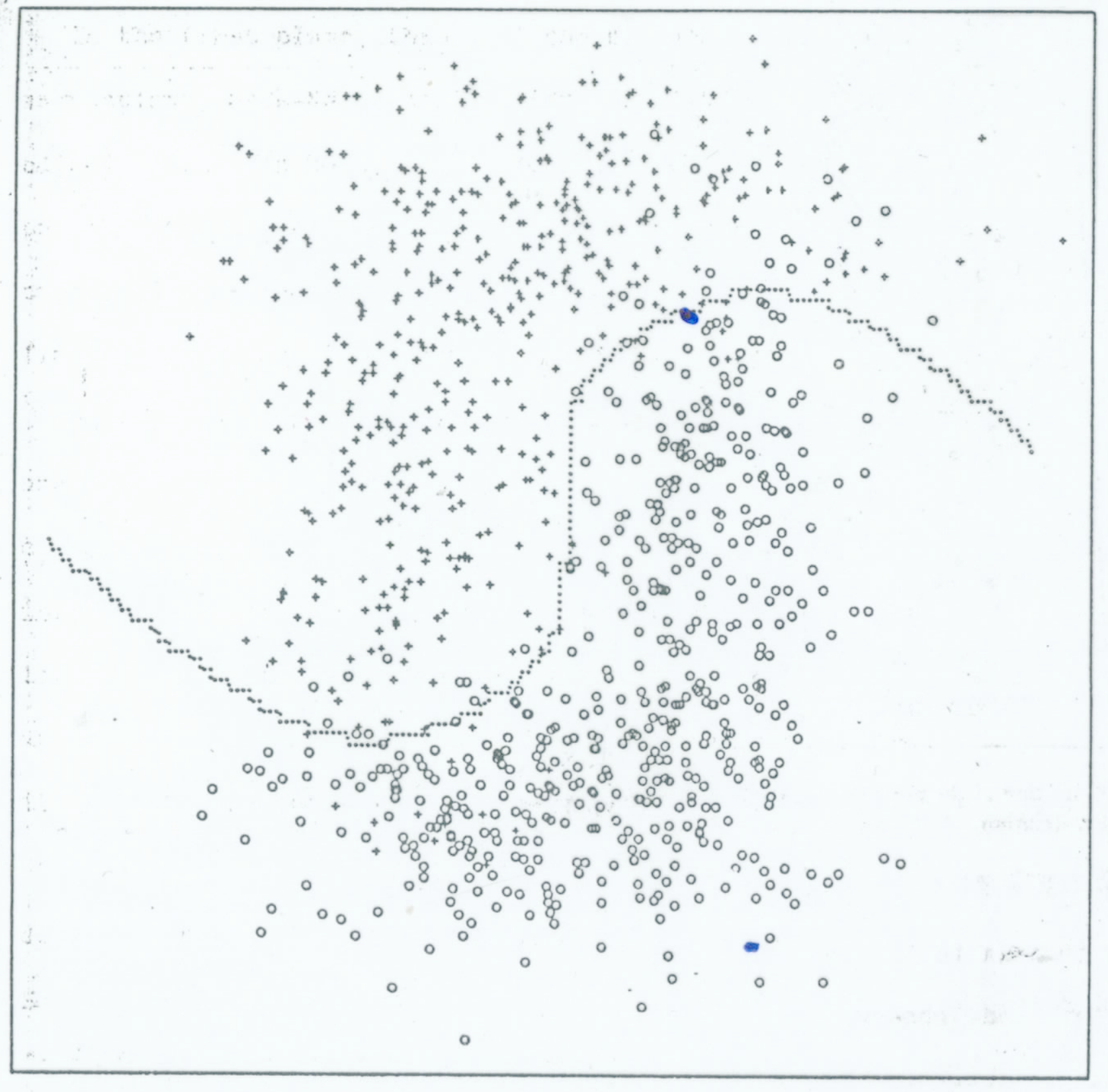


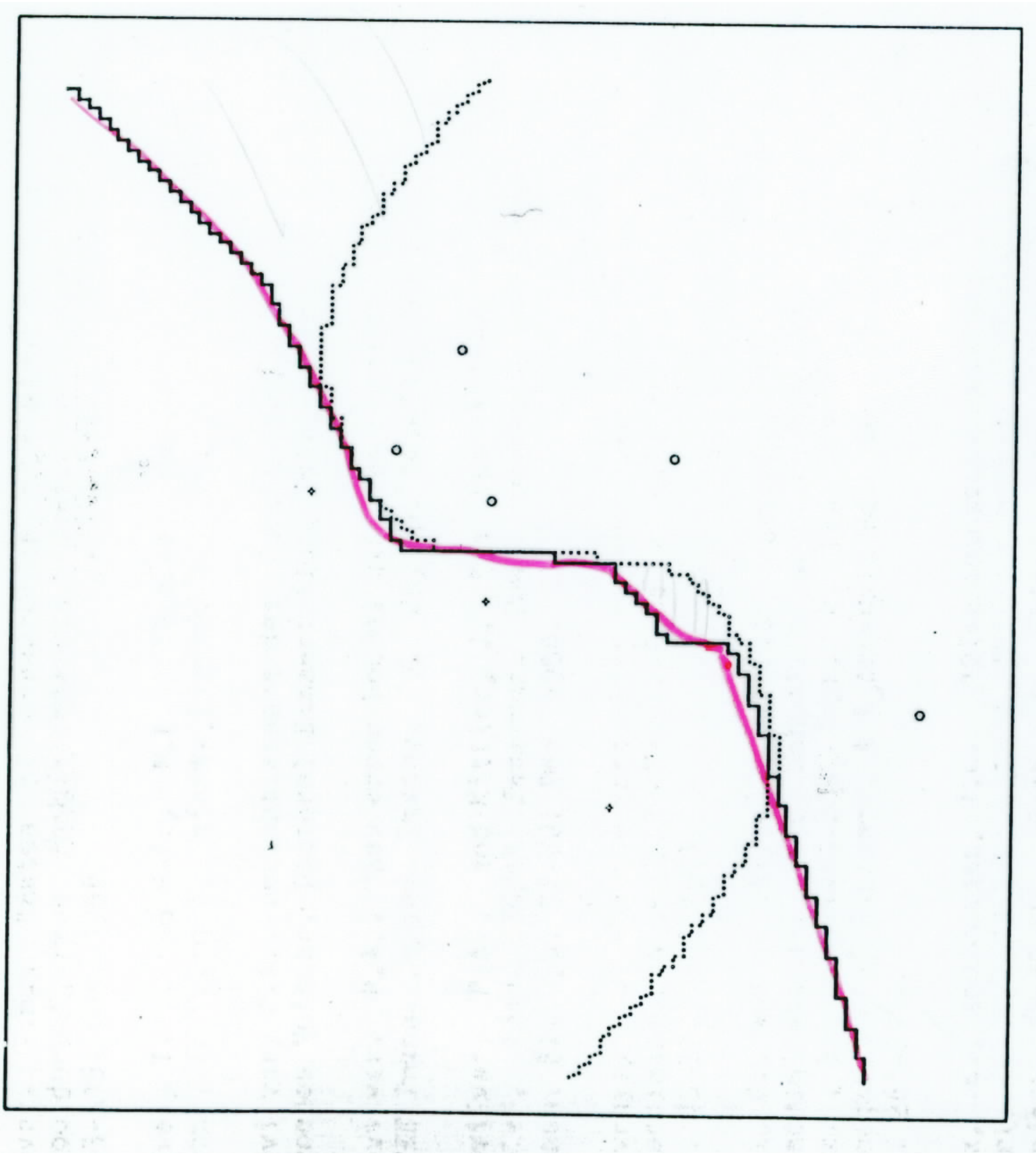
NN classification, K = 5

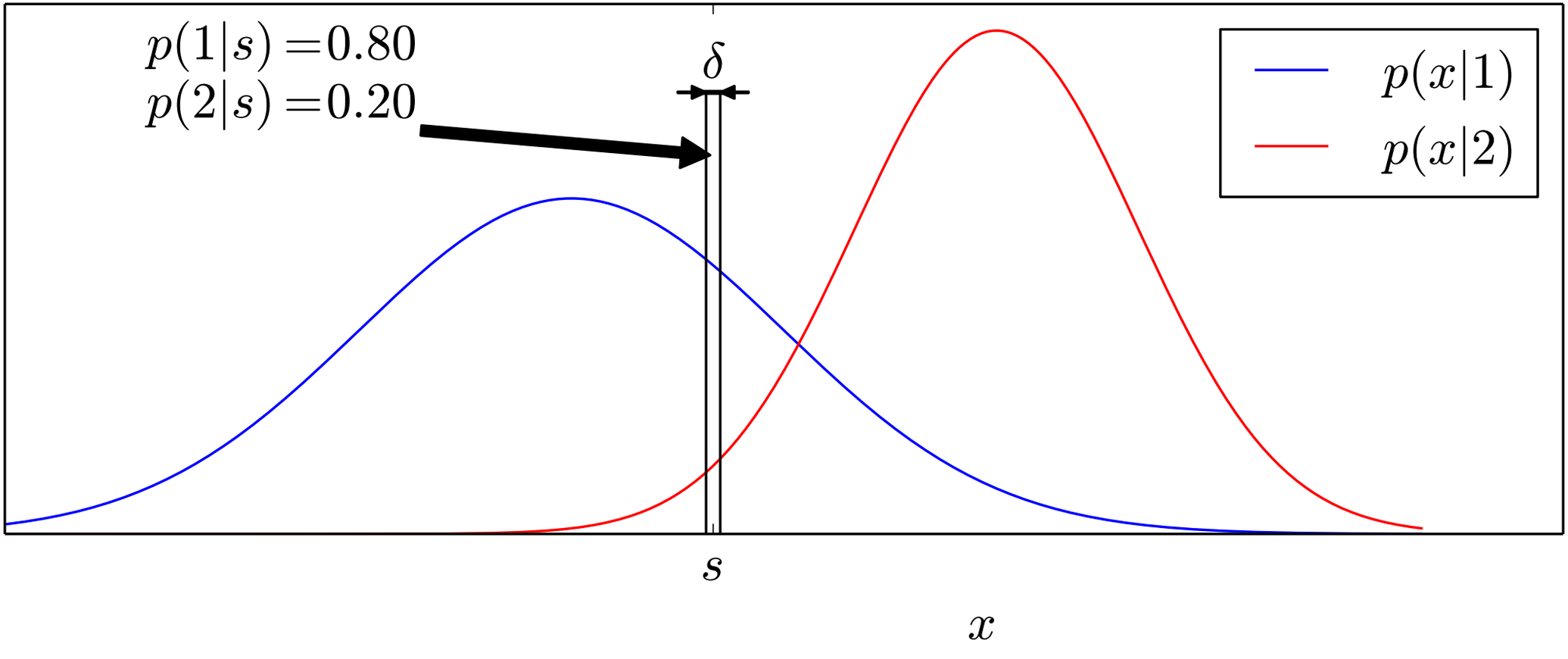


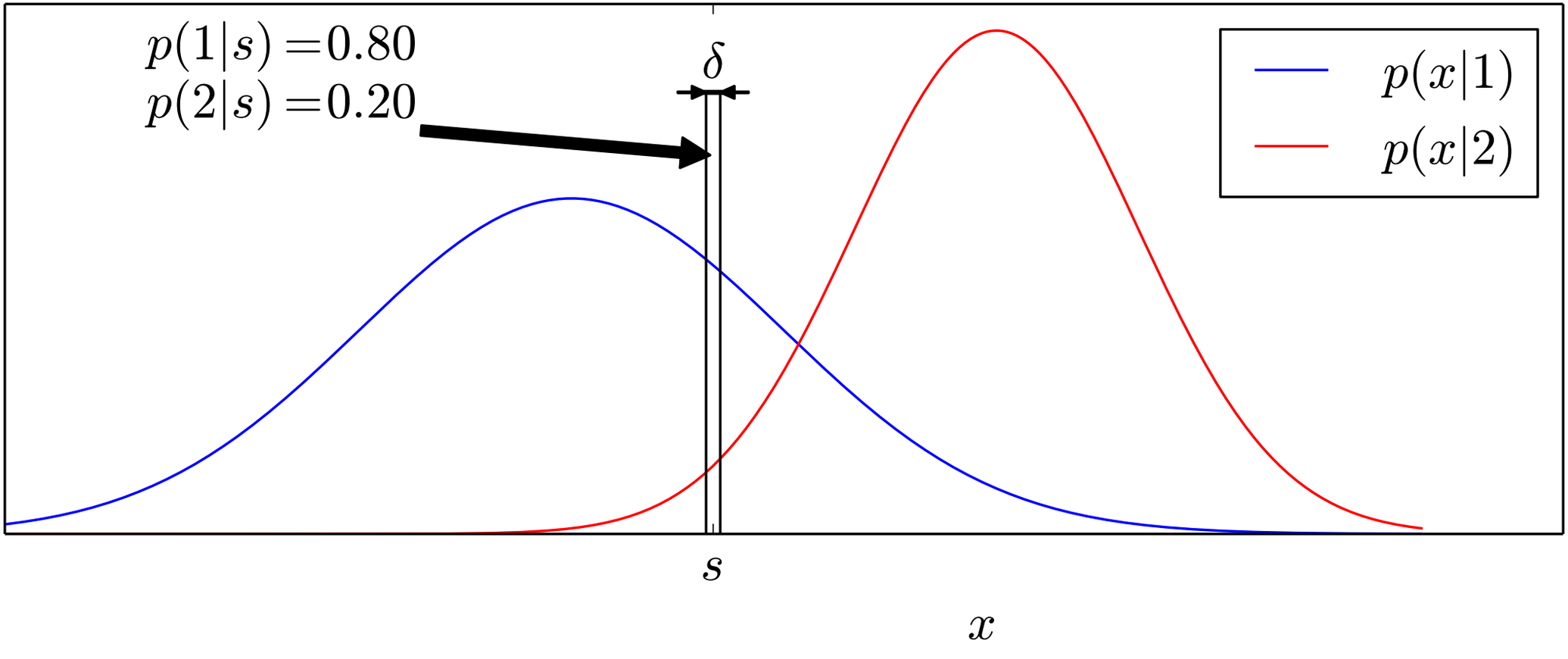
NN classification, K = 7

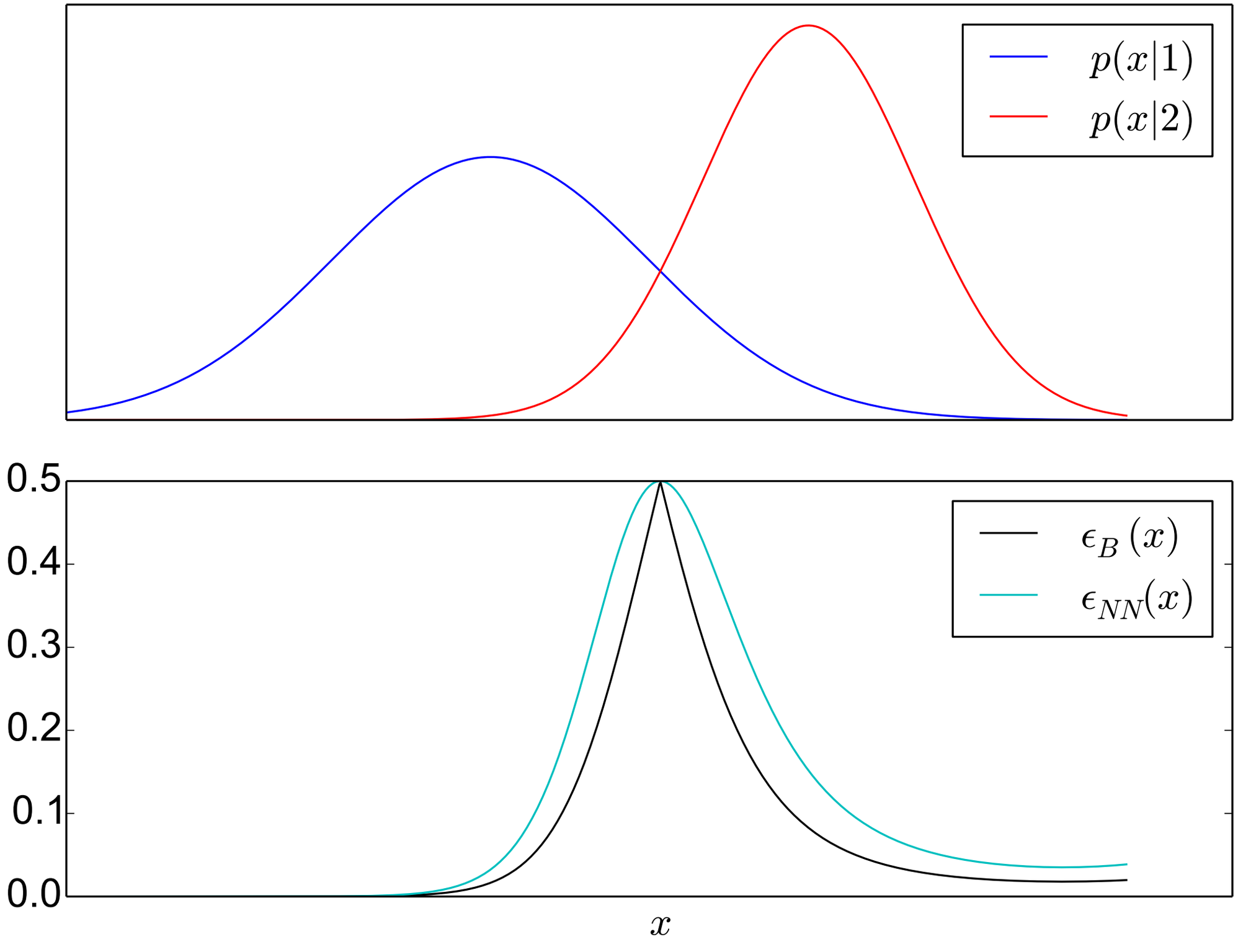







$p(1|s) = 0.80$
$p(2|s) = 0.20$
δ
$p(x|1)$
$p(x|2)$
s
x


$p(1|s) = 0.80$
$p(2|s) = 0.20$
δ
$p(x|1)$
$p(x|2)$
s
x


$p(x|1)$
$p(x|2)$
0.5
0.4
0.3
0.2
0.1
0.0
$\epsilon_B(x)$
$\epsilon_{NN}(x)$
x